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Front cover: Dan Oron



Dear Readers,

Despite the ongoing war, we welcome you to the eleventh issue of the Israel Chemist and Engineer (ICE) online magazine, a publication of the Israel Chemical Society (ICS). We hope you will find the magazine interesting and will be inspired to contribute to future issues.

We present three scientific reports on diverse topics from recent ICS prize winners: Roi Baer, the recipient of the 2024 ICS Excellent Scientist Prize has contributed an article on “ ,” Joshua Baraban, the recipient of the 2024 ICS Excellent Young Scientist Prize, has contributed an article on “Spectroscopy of reactive molecules,” and Dan Oron, the recipient of the 2024 Tenne Family Prize for Nanoscale Sciences, has contributed an article on “How avalanche photodiode array technology is transforming the spectroscopy of multiply excited quantum-dot emitters.”

We also present interviews with three outstanding Israeli scientists: David Avnir and David Cahen, recipients of the 2024 ICS Gold Medal, and Ilan Marek, the 2024 Richard Willstätter Lecturer. The Willstätter lecture is a joint venture of the German Chemical Society (GDCh) and the ICS, and the lecture takes place annually alternately in Israel and

Germany by either a German or Israeli lecturer. By a happy coincidence, Bob Weintraub has contributed a fascinating article entitled “Richard Willstätter (1872-1942), chlorophyll, and the three Goldschmidts.” Bob’s articles appear in every issue of the ICE magazine, and almost every issue since 2001 of its predecessor, Chemistry in Israel Bulletin.

In this issue, we continue our series of articles on potential careers for chemistry graduates, with Orit Ben Zazon on “CMC evaluation: ensuring quality in the pharma industry.”

If you have suggestions for future issues, comments on the current issue, or would like to contribute an article, please contact me at gordon@biu.ac.il.

Arlene D. Wilson-Gordon

Professor Emerita
Chemistry Department, Bar-Ilan University
ICE Editor



Dear Colleagues,

Over the past five years, our community has faced numerous challenges. Prior to October 7, 2023, we all believed that the COVID-19 pandemic had caused the most significant disruption to our personal and professional lives. Sadly, that belief was shattered by the shocking events that unfolded in the Middle East over the last two years. Many of our members have experienced loss, grief, and stress during this time, and a significant number of our students and young faculty have spent long months on active duty in the army.

Given this extraordinary background, the ICS recognized the importance of maintaining traditional scientific activities and providing opportunities for all Israeli chemists to gather, exchange information, and continue developing their professional careers. After a gap of 2.5 years between the 85th Meeting in February 2020 in Jerusalem and the 86th Meeting in Tel Aviv in September 2022, we faced challenges due to the consequences of the war, which forced us to postpone the 87th Meeting several times. Ultimately, we condensed it to a single day on April 3, 2024. The 88th Meeting, scheduled for February 18–19, 2025, at the ICC in Jerusalem (as detailed in my conference report in this issue), reflects our desire to return to a regular schedule. We are now looking forward to the upcoming 89th Meeting on February 10–11, 2026, at the Smolarz Auditorium in Tel Aviv University, under the leadership of Professors Yuval Ebenstein and Roey Amir.

The past two years have been challenging for me, as I have served as IUPAC President alongside my responsibilities with the ICS, the Israel Journal of Chemistry, and the Wolf Foundation. One of my flagship initiatives at IUPAC is the Presidential Prizes. Each prize is awarded annually by the IUPAC President, and the winner delivers a plenary lecture at either the World Chemistry Congress (WCC) or the EuChemS Chemistry Congress (ECC). <https://www.degruyterbrill.com/document/doi/10.1515/ci-2025-0101/html>

In July this year, during the 50th World Congress of Chemistry in Kuala Lumpur, I presented the inaugural IUPAC-Soong Prize for Sustainable Chemistry, which includes a \$30,000 award and a medal, to Professor Omar Yaghi. Five months

later, he went on to win the 2025 Nobel Prize in Chemistry. I encourage you to consider nominating deserving candidates for the 2027 cycle. <https://iupac.org/2026-iupac-soong-prize-for-sustainable-chemistry-call-for-nominations/>

During these tumultuous times, many positive developments have occurred. We have signed an agreement with the German Chemical Society regarding the Richard Willstätter Lectureship. A unique aspect of this scientists' exchange program is that each traveling scientist will bring an exceptional graduate student with them. We are also developing similar exchange programs with the Chemical Society of Japan and the Taiwan Chemical Society. These new agreements complement the five collaboration agreements we previously signed with organizations in the USA, Germany, Spain, the Netherlands, and the Czech Republic. Additionally, the ACS Israel International Chemical Sciences Chapter continues its activities under the leadership of its new president, Mindy Levine, along with Secretary Anat Milo and Treasurer Jonathan Church.

Another sign of our return to a regular schedule is the resumption of activities by our ICS Sections. The Bioinorganic Chemistry Section is led by Graham de Ruiter, Omer Yehezkeili, and Amir Mizrahi, while the Organic Chemistry Section is under the leadership of Doron Pappo, Mark Gandelman, and Elad Shabtai. The Organic Chemistry Section will hold its annual meeting on June 25, 2026, at the Technion. During this event, we will award the inaugural 2025 ICS-Richard A. Lerner Memorial Prize. The recipient, Prof. Véronique Gouverneur from the University of Oxford, will be honored for her pioneering work in organic synthetic methods and her significant contributions to the synthesis of organofluorine compounds, which are vital to medicine, agriculture, and materials science. I want to take this opportunity to thank the contributors to the prize endowment (\$100,000): Professors Phil Baran, Benjamin F. Cravatt, Jeff W. Kelly, Chi-huey Wong, and Jin-quan Yu from TSRI, as well as Dr. Phillip Frost.

Finally, we encourage you to help develop the ICE magazine under the leadership of Prof. Arlene Wilson-Gordon. We invite you to contribute an article on any topic that resonates with you, including popular science, the history of science, reports on events, opinions, and more. Your unique perspective is valuable to us. Please feel free to reach out to Arlene or me with any questions or ideas.

Enjoy your reading,

Ehud Keinan

President, the Israel Chemical Society

On building bridges: scientific cooperation as diplomacy of trust

Address at Opening Session of TU Berlin-Israel workshop on “Carbon Dioxide Valorization”, September 1, 2025

Helmut Schwarz

Honorary President of the Alexander von Humboldt Foundation

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Shalom and a warm welcome to TU Berlin!

In an address commemorating the beginning of World War II on September 1, 1939, George Santayana remarked that “Those who forget the past are condemned to repeat it.” These wise words of the distinguished Harvard scholar may well have served as the guiding principle of two political giants of the 20th century, the German Chancellor Konrad Adenauer and the Israeli Prime Minister David Ben-Gurion who, more than 65 years ago, out of the ashes of the Second World War, initiated the establishment of diplomatic relations between Israel and Germany.

For many good reasons, most Israeli citizens criticized and mistrusted the establishment of these relations. In fact, they viewed any of these and related initiatives as highly immoral. After all, survivors of the extermination camps would never ever forgive or could be possibly expected to forget these dark, evil days of German history.

Nevertheless, the two political leaders acted as philosophical prophets and, in an extremely courageous way ignoring personal risk and working against the strong opposing current of public opinions which prevailed in their home countries, prepared the ground for the signing on May 12, 1965 of a document which officially established diplomatic relations between the two states. This date marked a truly rare miracle in the too often cruel history of mankind.

How did it all come about? History tells us that Jewish philosophers, writers, poets, lawyers, business men, composers, actors, medical doctors, musicians, scientists and so on, all played a pivotal role in the economic, cultural and scientific blooming of Germany prior to the Nazi regime. Therefore, in the late fifties of the last century, culture, science, and social programs were suggested as the foundation on which to base and eventually renew relations across political

Helmut Schwarz read chemistry at the Technische Universität Berlin (TUB) from 1966–1971. After completing his PhD in 1972 under the supervision of Ferdinand Bohlmann and his Habilitation in 1974 (both at TUB), he spent some time abroad (ETH Zürich, MIT Cambridge, and Cambridge University) before returning in 1978 to his alma mater to join the Institute of Chemistry. He has occupied visiting positions at 15 academic institutions world-wide, has delivered more than 1000 invited or named lectures and published > 950 peer-reviewed articles dealing with various aspects of gas-phase chemistry and physics. He has received close to 50 awards, distinctions, and honors from a dozen countries. After having served from 2001–2007 as Vice President of the German Research Foundation (DFG), in January 2008, Dr. Schwarz was appointed President of the Alexander von Humboldt Foundation.



divides, thus building bridges between the two countries in the aftermath of the Nazi era.

At its rather difficult beginning, this huge challenge was taken up by individuals in each country, and it was due to their untiring efforts, their determination and personal courage, that the ground was prepared for this unparalleled undertaking.

Scientific co-operation and the international exchange of young scientists were seen as the most promising means by which frontiers, and not just proverbial walls, might be overcome. And, who would have dared to think in the early fifties, when Germany's and Israel's shared past was still so bleak and burdened, and when the experience of extermination, displacement and genocide, was still so vividly present among the survivors of the Shoah, that the sheer concept of a shared future, developing out of individual scientific co-operation, was more than a naïve dream? Who would have dared to predict, that seven decades later, the German-Israeli relationship due to the fine work of the exceptional Minerva Stiftung and the superb GIF and DIP programs, just to mention a few of the main players, could be recommended as a role model and celebrated as a huge success story of which we have good reason to be proud today?

How did all this come about? A possible explanation can perhaps be provided by briefly mentioning just one example from the rich history of the Alexander von Humboldt Foundation.

Right back in 1958, seven years before diplomatic relations between Israel and Germany were established, the first Humboldt research fellow from Israel arrived in Germany, a young woman, a lawyer from the Hebrew University of Jerusalem. As a postdoctoral fellow, she spent 20 months working on "International Law" at the University of Frankfurt am Main. What a brave and courageous step, and what great a human gesture! Can we really imagine the rather mixed feelings of a person coming to Germany, living in a country whose inhabitants and political leaders only a few decades ago were determined to exterminate all Jewish life? My admiration for that woman, Dr. Eva Shachor-Landau, as well as for Dr. Israel Pecht, a physical chemist from the Weizmann Institute, who joined Manfred Eigen's laboratory in Göttingen in 1960—my admiration for these pioneers of friendship is boundless.

While Dr Shachor-Landau was the first Humboldt fellow from Israel, many followed her to spend extensive periods in Germany. Since 1958, a total of close to 250 postdoctoral students have come from Israel to Germany, and the Humboldt Stiftung has also granted 145 prestigious Humboldt Research

Awards to Israeli scientists and scholars including Nobel Laureates and similarly distinguished individuals – this number is, per capita, the by far highest number worldwide and speaks for itself about the quality of academic life in Israel. Further, the exchange of scientists was not a one-way affair because a significant number of young German scholars also spent their formative years in Israeli academic institutions sponsored by the various scholarship programs. At the institutional level, there was the door-opening, legendary (and secret) flight of the Max Planck scientists Otto Hahn, Wolfgang Gentner and Feodor Lynen on December 1, 1959, from Zurich to Tel Aviv at the invitation of the Weizmann Institute of Science. It was this semi-official, somewhat "private" meeting of German and Israeli scientists in Rehovot which encouraged Adenauer to continue his difficult dialogue with Ben-Gurion and which, a few years later, led to the foundation of the incredibly successful MINERVA Stiftung. No doubt, all these and many other scientific activities have contributed enormously to the standing and reputation of the two countries and have enriched both the personal and professional lives of numerous human beings, including myself. In my own, rather long academic life, I have visited Israel around 125 times.

However, this extraordinary growth of friendship and trust did not come about on its own accord in the past, and, most importantly, cannot be taken for granted in the future either. Co-operation and solidarity depend crucially on continuing efforts being made by both sides; trust has to be established time and again, and social bonds need to be cultivated constantly and sustainably as is the need to irrigate a garden in the desert.

Tackling critical, often painful issues, and engaging in disputes including politically sensitive questions as, for example, the appalling policy of the present government in Jerusalem, are all part of the package. There exists no royal road that bypasses obstacles, and exclusive reference to a common history is not sufficient to serve as a reliable basis for building a joint future.

In the past, the academic co-operation between Israel and Germany has convincingly demonstrated how science can act as a tool for a diplomacy of trust, can open channels between adversaries, provide a refuge for dialogue in times of political rupture and thus bridge separated domains, can help to overcome bitter experience and memories, and bring collective knowledge across disciplines and cultures to bear on developing solutions to quite intractable challenges. However, over the last few years, we have increasingly witnessed politically and ideologically motivated efforts to boycott Israel at large, including Jewish individuals and Israel's fine academic institutions. While the latter constitute

true liberal fortresses in an unfriendly, if not hostile, political environment, its politically requested boycott will only weaken these liberal forces which are so badly needed. As such acts, often internationally coordinated by BDS-activists, also endanger academic freedom and are an assault on free speech and human rights, all of us should unite against the destruction of these basic values and the foundations of academic life. Clearly, it may be needless to stress that we owe the same decisiveness in protecting the rights of others, including Palestinian inhabitants of the West Bank and Gaza. It is my firm conviction that Israel and Germany seek future academic, cultural and political co-operation with all like-minded, good-mannered, benevolent partners from all over the world, for the sake of everyone. Building and shaping a shared future will not be possible without co-operation, regardless of how difficult and demanding this project may look like for the time being. Around 600 years ago, when the “black death” plague took its heavy toll in Europe and the political situation was frighteningly unstable, in a season of terror and death, Dante Alighieri noted in his diary that “one day the stars will shine again” – and history proved him right.

The often-quoted words “Anyone who does not believe in miracles is not a realist” are attributed to Israel’s first Prime

Minister, the legendary David Ben-Gurion. I should like to encourage you to dream such dreams – and be such a realist: Be motivated by what has been achieved so far, be encouraged by the unexpected success stories, do not mind to show empathy for your opponent’s position and don’t be afraid and demotivated by the obstacles you are likely to encounter, get yourself involved in securing a common future and play a role in facilitating responsible science and togetherness shaped by trust and optimism.

Dear friends and colleagues, let us not forget: co-operation helps bind us as a community as it did in the past and, hopefully, will do in the future. Wilhelm von Humboldt, the intellectual father of the modern Research University, once remarked: “Only he who knows the past has a future,” and these words hold true even after 200 years, and both the Israeli-German reconciliation and the numerous institutional and personal bonds have indeed set the stage for better years to come.

Herzlichen Dank and Rav Todot.

Richard Willstätter (1872-1942), chlorophyll, and the three Goldschmidts

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Abstract

Richard Martin Willstätter (1872-1942) was a pioneer of organic and biological chemistry. In 1915 he was awarded the Nobel Prize in Chemistry for research on plant pigments, especially chlorophyll. Willstätter was born in Germany into a Jewish family. Antisemitism and a love of his native Germany were determining factors of his career and life. In 1924 he resigned his academic position at the University of Munich in protest against antisemitism at the University. At that time, three faculty positions became available at Munich, but the worthiest candidates were not offered the positions because they had Jewish ancestry. By coincidence, the surname of all three was Goldschmidt: the organic chemist Stefan Goldschmidt (1889-1971), the geneticist Richard Benedikt Goldschmidt (1878-1958), and the geochemist Victor Moritz Goldschmidt (1888-1947). In 1934 Willstätter came to Palestine to deliver the opening address of the Daniel Sieff Institute, in Rehovot, which was the beginning of the Weizmann Institute of Science. He returned to Germany. Despite German antisemitism and being offered positions all over the world, Willstätter refused to leave his beloved Germany. In 1939 the Gestapo came to his home in Munich with orders to transfer him to Dachau; it was then that Willstätter escaped Germany to Switzerland.

Introduction

D. Nachmansohn: “Richard Willstätter was one of the giants in organic chemistry who, at the turn of the century, had laid the foundation for the spectacular developments of biochemistry in the century. He belongs to the extraordinary and ingenious group of Adolf von Baeyer’s pupils, who paved the way for a new era in biological sciences by providing the knowledge of the structure of the most essential components of animal and plant cells, a prerequisite for the analysis and understanding of chemical cell reactions.

“One of his most brilliant contributions was his work on the structure of chlorophyll; it is one of the classic works in organic chemistry. His many achievements in solving this problem were summarized in collaboration with his associate Arthur Stoll in *Investigations on Chlorophyll* (Willstätter

and Stoll, 1913). These contributions are a milestone in the exploration of photosynthesis. For this work and for his investigations on the structure of pigments of flowers and fruits, the anthocyanins, he received the Nobel Prize in 1915. His lifework was of great importance not only for biochemistry, but also for medicine and technology” [1].

In 1939 Willstätter escaped his native Germany. He wrote his memoirs in exile and completed them in 1940. He wrote, “Certain chemical observations early in my career determined the course of my life—in particular, a discovery concerning the behavior of the methiodide of tropic acid ether. The currents and later the tide of anti-Semitism were equally influential. No matter how diverse, the decisive factors must fit into a single framework” [2]. His memoirs begin with the words, “My forefathers were Jews.” See Figures 1-3.

Bob Weintraub was born in Brooklyn, New York and made aliyah in 1975 to Beer Sheva, where he remained. He earned the PhD in Physical Chemistry from MIT and the Diploma in Library Science from the Hebrew University of Jerusalem. He held positions in scientific and technical librarianship in industry, hospital and academic institutions. He is now retired. He has an interest in the history of chemistry.



Chlorophyll

Richard Martin Willstätter (1872-1942) together with his collaborators studied and worked out the structure and syntheses of tropine alkaloids—including cocaine and tropine; elucidated the structure and synthesis of cyclooctatetraene; studied the quinone and quinone imines, the Wurster dyes, and aniline black; investigated chlorophyll and haemoglobin; worked out the structures of the blue, red and violet anthocyanins—and synthesized cyanins, flavones, and pelargonidin; studied the yellow carotenes, and other pigments of fruits and flowers. They studied the nature of photosynthesis, the chemical composition of plant and animal enzymes, and the assimilation of carbon dioxide in plants. See Figure 4.

The determination of the structure of chlorophyll took ten years to accomplish. Prof. O. Hammarsten, Chairman of the Nobel Committee for Chemistry: “The most important part of Willstätter’s investigations is, nevertheless, that relating to the detection of the chemical structure of chlorophyll. He has shown that chlorophyll is an ester, which on saponification with alkali can be split up into a previously unknown alcohol called ‘phytol,’ which represents about one third of the molecule, and a color component called ‘chlorophyllin,’ containing magnesium, which forms the remaining part. He has more closely investigated these two components both individually and for their transformation and decomposition products. Furthermore, he has found that this splitting-up of chlorophyll into the two mentioned main components can also take place as a result of the action of an enzyme occurring in the leaves, which he has called ‘chlorophyllase,’ and hence he has been able to elucidate the nature of the crystallized chlorophyll. He has established that this is not, as some investigators have assumed, the pure, unchanged natural pigment in the leaves. The crystallized chlorophyll is a laboratory product, an alkyl ester, which lacks phytol. The amorphous chlorophyll, containing phytol, is the unchanged natural pigment in the green parts of the plant.

“In these investigations, which concerned pigment nucleus both in chlorophyll and in haemoglobin, he has made several new and important observations regarding the pyrroles and their position in this nucleus; in particular, however, he has shown that from these two pigments the same parent porphyrin, ‘aetioporphyrin’, can be prepared, whose molecule has retained the essential characteristics of the pigment nucleus. By doing this he has produced the most interesting and decisive proof of the relationship between the two most biologically important pigments in Nature, haemoglobin and chlorophyll” [3].

Nobel prizes on the structure of chlorophyll and anthocyanins

In addition to the award of the Nobel Prize to Willstätter in 1915, four later Nobel awards for chemistry were also related to the structure of chlorophyll and anthocyanins: Hans Fischer (1930), Paul Karrer (1937), Robert Robinson (1947), and Robert Burns Woodward (1965).

Hans Fischer was awarded the 1930 Nobel Prize in Chemistry for his researches into the constitution of haemin and chlorophyll, and especially for the synthesis of haemin. Nobel Prize website: “Structural similarities between haemoglobin and the plant pigment chlorophyll had been uncovered by the 1915 Chemistry Laureate Richard Willstätter, when he showed that chlorophyll holds an atom of magnesium within the centre of the molecule in the same way in which iron is held within haemin. Fischer provided a more detailed view of this similarity when he showed that chlorophyll is constructed from the same pyrrole constituents that make up haemin” [4].

Willstätter credits **Paul Karrer**, who shared the 1937 Nobel Prize for investigations on carotenoids, flavins, and vitamins A and B2, for improvements and supplementary work in the elucidation of the anthocyanins. Karrer, in his Nobel lecture, said that progress in methods which modern biochemistry can no longer dream of doing without include the selective adsorption processes of Willstätter [2] [5].

Arne Westgren, Secretary of the Royal Swedish Academy of Sciences, considered that **Robert Robinson**, who was awarded the Chemistry Prize for 1947 for his investigations on plant products of biological importance, especially alkaloids, “may also to a certain extent be looked upon as a successor to Willstätter.” Robinson carried out work on the colored anthocyanins common in the plant world, in addition to works in a much wider field [6]. Willstätter: “The comprehensive elucidation of the glycosidic anthocyanins and the more complex phenomena of natural flower colors by Mr. and Mrs. Robinson, the structural determinations and synthesis with new methods, not only of the aglycones but also the much more difficult ingenious syntheses of natural glycosides— these were problems and achievements of great significance. I regard it as my good fortune to have witnessed this elegant and profound consummation” [2].

Robert Burns Woodward was awarded the 1965 Nobel Prize in Chemistry for his outstanding achievements in the art of organic synthesis, notably the total synthesis of chlorophyll [7]. Woodward, in referring to Willstätter, “That great investigator isolated the pigment [chlorophyll a]—and its closely related frequent minor concomitant chlorophyll b as well—in the

pure state, established correctly the empirical formula of the substance, and laid down a sound and extensive preliminary basis of transformation and degradation. Half a century of structural study culminated in the complete formula for chlorophyll a. These achievements can be measured against the fact that the isolation of chlorophyll in a state of purity is even now, after more than fifty years, no mean feat, and, further, that the empirical formula defined by Willstätter, repeatedly called into question by subsequent investigators, has stood the test of time” [8].

“Einstein is a German Jew; I am a Jewish German.”

Willstätter studied in Munich at the Technische Hochschule and University. He was awarded his doctorate in 1894 for work on the structure of cocaine. He stayed at the University in Munich until 1905, at which time he accepted a professorship in Zürich at the Swiss Polytechnic Institute. In 1912 he returned to Germany to Berlin-Dahlem and in 1915 accepted the chair in Munich as successor to his revered 80-year-old mentor Adolf von Baeyer, who was retiring from teaching. He rose to the position of dean of the faculty. Willstätter’s return to Germany was motivated by his deep feeling of being a German and of wanting to return to his homeland. Years later, after his resignation from Munich, he elaborated to Sir Robert Robinson on these feelings by saying, “Einstein is a German Jew; I am a Jewish German” [9].

Willstätter: “In the years of my instructorship the friendship which Baeyer showed me and which was the greatest human experience of my youth unfortunately declined. When I published papers in *Berichte der Deutschen Chemischen Gesellschaft* one and two years after my qualification, Baeyer remarked, ‘Now you’re in.’ And both times he added the advice, ‘But you must let yourself get baptized.’ How grateful I was to him that he had suggested qualification with no strings attached! The advice was brief and so was my answer, perhaps a little too bluntly worded. The connection with a career was repugnant to me. Coming from the great man whom I could not suspect of opportunism, the suggestion was incomprehensible to me. I came to understand him, finally, much later.”

Baeyer belonged to a Jewish family where baptism and intermarriage were acceptable and common. Conversion removed the barriers to a career and to absorption into the leading stratum of society. Willstätter explained that he and Baeyer came from different circles of the German Jewish community. For Willstätter, raised in a more provincial circle, that path involved emigration. Willstätter: “Whereas assimilation was the maxim familiar to him through experience, Judaism meant history to me. Conversion seemed

improper to me without religious reasons, especially so if it was combined with personal advantage” [2].

Three Goldschmidts

In 1924, three faculty positions became available at the University of Munich. The worthiest candidates were not offered the positions because they had Jewish ancestry. By coincidence, the surname of all three was *Goldschmidt*. [10]

The organic chemist **Prof. Stefan Goldschmidt (1889-1971)** from the Technische Hochschule in Karlsruhe was Willstätter’s choice for the position to replace Prof. Pummerer, who moved to Greifswald. In 1938 Prof. S. Goldschmidt found refuge in Holland, where he was associated with the pharmaceutical industry. After the war he returned to the University of Munich as Professor of Chemistry and Director of the Institute of Organic Chemistry, from which he retired in 1957.

Prof. Richard Benedikt Goldschmidt (1878-1958) of the Kaiser Wilhelm Institute of Biology was considered for the position to replace retiring Professor Richard von Hertwig, the geneticist. Hertwig did not propose Goldschmidt, and explained to Willstätter, that for many years it was his dearest wish to have Goldschmidt as his successor, but that the currents of the time had made it impossible. Hertwig: “We do have to take the times into account, and defer to popular opinion.” R. B. Goldschmidt found refuge in the United States and accepted a position in 1936 as Professor of Zoology at the University of California at Berkeley. He remained at Berkeley for the rest of his life [11].

The retiring Prof. Paul von Groth had always maintained that the only person suitable to succeed him was the geochemist **Prof. Victor Moritz Goldschmidt (1888-1947)**, from the University of Oslo. V. M. Goldschmidt is recognized as *The Father of Modern Geochemistry*. He was not offered the position. He later accepted a position in Göttingen and seven years later fled to Norway. After the German invasion of Norway, Goldschmidt was twice arrested and sent to the Berg Concentration Camp, on the outskirts of Tønsberg. The second time, Goldschmidt was rescued from the pier at Oslo harbor as he was about to board the prisoner ship *Donau*, bound for Auschwitz via Stettin. With the help of the Norwegian resistance, Goldschmidt was taken to Sweden, and from there found refuge in England and Scotland. His health was in ruins due to the treatment that he experienced at the hands of the Germans. In 1946 he returned to Norway [12].

Resignation

Chaim Weizmann, who had great respect for Willstätter, described what happened next, “At a meeting of the (Munich)

University senate some time in 1924 a discussion had arisen about the appointment of a mineralogist. A candidate was proposed, a front-rank mineralogist by the name of Goldschmidt. As soon as the name was mentioned a murmur arose in the meeting and someone remarked: *Wieder ein Jude!* (another Jew). Without saying a word Willstätter rose, collected his papers and left the room.” Willstätter remained in office only long enough to aid his students to complete their researches and to make the installation of his successor, Prof. Heinrich Wieland, as smooth as possible. Weizmann: “(Willstätter) never crossed the threshold of the University again, this despite the repeated entreaties of his colleagues and of the Bavarian Government. It was felt—this was still 1924—that he was too valuable a man to lose and his withdrawal was a severe blow to the prestige of the University” [13].

Heinrich Wieland thought that Willstätter had been wrong in resigning. In 1924 Wieland wrote to Willstätter, “You should put the welfare of our field ahead of personal annoyance and conviction. You are also completely wrong in your ideas about anti-Semitism. There is no anti-Semitism of any consequence in Germany” [2]. Willstätter selected Wieland as his successor and persuaded him to accept. In 1927 Wieland was awarded the Nobel Prize in Chemistry for his investigations of the constitution of the bile acids and related substances [14].

Soon after his resignation, Willstätter was led by surprise to a meeting by two colleagues, to find a room filled with colleagues from the institute, his assistants, and students. A letter and address signed by 377 names was presented to him, in part, “We see in you the rare personality of a leader to whom all of us, without exception, look up to as an unattainable example, and we are deeply disturbed by the thought that you wish to abdicate your leadership. In this time of our country’s deep humiliation we young people feel the want of leaders, of examples, of pure, good men so keenly that we cannot do without the few we have. You, honored Sir, are one of the few, and we beg of you most earnestly to make what may be the biggest sacrifice of your life, and to remain our leader.” The students ended their letter with the sentence, “Now we feel we must make manifest to you, Sir, not only our unreserved trust, but our admiration and the solemn promise of our loyalty as well” [2].

Felix Haurowitz was present at that meeting. Haurowitz worked in Willstätter’s laboratory in the summer of 1924. In 1978 he recalled the historic event, “At this convention Willstätter thanked the students and made the declaration—in his measured tranquil way of speaking—that he had no intention of staying with a Faculty in which Professors make decisions on candidates for vacant chairs not on the basis of qualifications but race. He then slowly rose and—without looking left or right—slowly moved out of the lecture hall. As

this happened, all the students rose. Nobody said a word, while Willstätter slowly left. It was like a funeral” [15]. Haurowitz, who was Jewish, fled Nazi occupied Europe finding refuge first in Turkey and later in the United States [16].

Willstätter’s resignation attracted much attention and he was offered positions all over the world, including Germany and the United States. He took none of these into consideration as he did not want to make the affair into a matter of career or change of position. Willstätter was 53 years old.

Willstätter wrote in his memoirs (completed in 1940), “A single such fate, a non-Aryan’s departure from office, has become quite natural and unimportant. Nevertheless I must tell the story; the picture of the tolerant, liberal, just spirit which predominated such a short time ago and which seemed ineradicable deserves to be recorded along with the departures from it; for since my own isolated, early case the transformation in captive public opinion, in the students’ emotionalism and the professors’ opportunism, and in the measures taken by the authorities and learned societies in Germany on orders from above, has been uniform and complete. A number of other countries also quickly imitated these reactionary phenomena. ‘The more things happen in quantity and we deal in multitudes, the more will the workings of human thought be impeded. And the nations will have to pay for their mistakes in blood’ [Rahel von Varnhagen]” [2].

Chaim Weizmann: “For a long time Willstätter refused—in spite of his experience in 1924 and his violent reaction to it—to understand what was taking place in Germany. I saw him in Munich, at the end of 1932, and again in Zurich and Paris, in 1933, after Hitler had come to power; but, though deeply disturbed, he would not believe that the German people and the government would go any further in their anti-Jewishness. We discussed the Daniel Sieff Research Institute, which was then in process of construction; he was immensely interested and generous with his advice. He readily accepted my invitation to preside at the opening, but to my repeated and insistent pleas that he leave Germany and come to us in Palestine, he turned a deaf ear. He came to the opening of the Institute and returned to Germany (in 1934!). He still felt that he was protected by his reputation and by the devotion of the Munich public.

“But nothing of all this induced him to change his mind. His last word on the subject was: ‘I know that Germany has gone mad, but if a mother falls ill it is not a reason for her children to leave her. My home is Germany, my university, in spite of what has happened, is in Munich. I must return.’ He actually stayed on in Germany until the outbreak of the war in 1939” [13].

On November 10, 1939, the Gestapo searched Willstätter's home looking for him, having orders to transfer him to Dachau. He escaped to Switzerland and settled in Muralto-Locarno. Here he worked on his memoirs. He died in 1942.

Willstätter recalled being elected in 1914, together with his close friend Prof. Fritz Haber, to membership in the Prussian Academy of Sciences. Willstätter attended regularly and sat next to Prof. Albert Einstein. Willstätter: "For twenty-five years I enjoyed membership in the Prussian Academy of Sciences as a regular member, then as honorary and finally foreign member. In some scholarly societies the president—appointed, not elected—endeavors all too sedulously to comply with or anticipate the new regulations. According to Plutarch, when Aristides was asked what he found hardest to bear in his exile, he answered, 'that my native land has dishonored itself so by my exile' " [2].

Inaugural address of the Sieff Institute

Willstätter delivered the inaugural address of the Sieff Institute on April 3, 1934, see Figure 5. In his address, he offered three pieces of advice: Investigate the products of this country and use the knowledge gained for the improvement of nature; Do not limit the research to applied work, but work

on subjects that may change the very basis of research and of science itself; Do not spread your research too wide and do not write many papers, "*Non multa – multum* [not many things – much; meaning not quantity – quality]" [17].

Willstätter: "The scholars of this institution should remember for what they are working – for something higher and greater than their own self-interest." Willstätter ended his talk with the words that he saw on the gates of the institute, "Work for this Country, Work for Science, Work for Humanity" [17].



Figure 2. Bust of Richard Willstätter, Bavarian Hall of Fame, Munich. E. Luttner, artist. Photograph by author.



Figure 1. Photograph of Richard Willstätter, with his signature. This photograph is on the desk at the museum of the restored laboratory of Dr. Chaim Weizmann at the Sieff Institute. Weizmann displayed two photographs on his desk, this one and one of Prof. Fritz Haber [18]. Original photograph by Müller-Hilsdorf. Image courtesy of the Weizmann Archives.



Figure 3. Memorial stone to German Jewish scientists in the courtyard of the Ullmann Building at the Weizmann Institute of Science*. The inscription is part of a sculpture called "Altars and Water Channels," by Buky Schwartz, 1963. The dedication reads, in English and Hebrew, "This institute stands as a living monument to Fritz Haber (1868-1934), Richard Willstaetter (1872-1942), Carl Neuberg (1877-1956), Otto Meyerhof (1884-1951), Max Bergmann (1886-1944), Rudolf Schoenheimer (1898-1941), and those German Jewish scientists who were victims of Nazi tyranny. Its creation was encouraged and supported by Chancellor Konrad Adenauer and the Max Planck Gesellschaft." Photograph by author.

* After this manuscript was submitted for publication, the Ullmann Building was destroyed on June 15, 2025, in an Iranian missile attack on the Weizmann Institute.

Spectroscopy of reactive molecules

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Abstract:

Abstract: Characterizing chemical reactions in depth requires spectroscopic techniques that can identify reactive molecules and follow their dynamics in extreme environments with quantum state resolution. Advances in this fundamental research area therefore involve improved understanding of the properties of reactive species and their interaction with light, hand in hand with development of new techniques that provide access to the chemical and physical details of reaction dynamics. Here I summarize some of our recent work on archetypal radicals, extreme environments such as high temperatures and plasmas, and novel spectroscopic detection techniques.

1. Introduction

The journey towards better understanding the processes of chemical reactions necessarily involves increasingly intrepid exploration away from equilibrium and low energy regions of phase space. Characterization of unstable and/or highly energized reactive molecules is a challenging task, especially in their native extreme environments, which demands continuing innovation in non-perturbative, and therefore typically spectroscopic, diagnostics. The reward is new fundamental physical and chemical knowledge that impacts many scientific and technological fields, leading to novel ways to monitor and control chemistry.

In this article, I will briefly survey some of the recent and ongoing work by my group and our collaborators on reactive molecules and development of appropriate spectroscopic methods for their investigation.

2. Radicals

Radicals are a principal class of reactive molecules. Their open-shell electronic structure poses several challenges, including chemical instability experimentally and vibronic coupling theoretically. Since radicals are frequently important reactive intermediates, and can also be considered the building blocks of molecules, overcoming these obstacles is often worth the considerable effort.

An illustrative example is our recent study of the cyclopropyl radical [1]. Cyclopropyl is one of the smallest cyclic radicals and serves as a fundamental instance of several important chemical phenomena, including ring strain, electrocyclic reactions, tunneling (involving flipping of the -H above and below the ring), and the strongest known C-H bond in cyclopropane due to the unusual hybridization. Surprisingly little direct experimental information is available on this

Joshua Baraban was born in 1983 in New York, NY, USA. He received his BS/MS in Chemistry from Yale University in 2006 with Prof. J. Michael McBride, followed by graduate work at MIT (PhD Physical Chemistry, 2013), on high resolution gas phase spectroscopic signatures of isomerization in the group of Prof. Robert W. Field. He was then a postdoctoral researcher with Profs. G. Barney Ellison and John W. Daily (CU-Boulder), where he developed an optically accessible pyrolysis microreactor. In 2017 he joined the Department of Chemistry at Ben-Gurion University of the Negev. The aim of his research is to develop spectroscopic techniques to characterize reactive molecules in their native, exotic environments, such as at high temperatures and in plasmas, revealing fundamental quantum aspects of these species' chemical properties and dynamics. Inherent in his group's efforts are both the design of novel sources for radicals and the pursuit of new (often laser-based) methods for their detection. Josh has won several research grants, including ERC Starting, NSF-BSF, Pazy, Ministry of Energy, and ISF; his list of awards includes the Alon fellowship for new faculty members (2019), the Krill prize for excellence in scientific research (2021), and the Toronto prize for excellence in research (2024). In 2024 he received the ICS Excellent Young Scientist Prize.



radical, and some of what is known is not yet fully understood. We reexamined the photoelectron spectrum of cyclopropyl radical using a combination of theory and experiment to shed new light on basic thermodynamic and kinetic questions surrounding the ring opening dynamics of the cyclic radical and cation (Figure 1).

Experimentally, the combination of several capabilities at the SOLEIL synchrotron in France was ideal for attacking this problem with modern methods: specifically an F atom abstraction reactor for *in situ* radical generation, synchrotron vacuum ultraviolet (VUV) radiation at the DESIRS beamline and the DELICIOUS3 double imaging photoion-photoelectron coincidence (*i*²-PEPICO) spectrometer. After production in the reactor, the C₃H₅ radicals – along with other by-products – are then irradiated by the VUV produced at the DESIRS beamline, leading to photoionization. The different chemical species present are then analyzed using the *i*²-PEPICO spectrometer, which associates the corresponding photoelectron spectrum with each species seen in the mass spectrum.

In addition, we theoretically modelled the theoretical photoelectron spectrum expected for the cyclopropyl cation, including its allylic form that results from ring opening, using an innovative calculation method [2]. Based conceptually on the Fourier transform of time-domain propagation of an initial state vibrational wavepacket on the final state potential, the calculation practically relies on an analytic expression for the autocorrelation function based on second-order vibrational perturbation theory, with potential force fields calculated by equation of motion coupled cluster methods. This hybrid approach that borrows from both time-domain and frequency-domain spectroscopy allowed us to systematically improve the accuracy of our simulation and match experiment even for this very challenging case.

These experimental and theoretical results were obtained by a collaborative effort between scientists at Ben-Gurion University of the Negev, Harvard-Smithsonian Center for Astrophysics, Institut des Sciences Moléculaires d'Orsay, Université Bordeaux, University of Florida – Gainesville, Argonne National Laboratory, and at the DESIRS beamline.

The comparison between experiment and theory provided refined values for the dissociation energy of the C-H bond in cyclopropane and the cyclization energies of cyclopropyl radicals and cations, among other important thermochemical quantities.

Finally, the close agreement between experiment and theory allows for the convincing conclusion that the cyclopropyl cation does not, in fact, exist as a stable species, but is

rather a transition state between allyl cation structures. The cyclopropyl radical then exists because of kinetic barriers to ring-opening, which are not present in the disrotatory opening of the cation. This settles a basic question going back to the early theory of pericyclic reactions (in which a molecule goes through a transition state with a cyclic geometry).

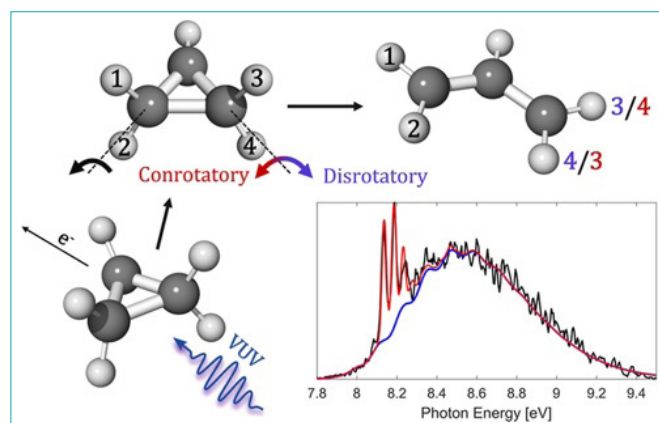


Figure 1. Depiction of the cyclopropyl radical undergoing vacuum ultraviolet photoionization followed by ring opening to the allyl cation. The experimental threshold photoelectron spectrum is compared to a sum of theoretical simulations for both cyclopropyl and allyl, derived from the Fourier transform of an analytic expression for the autocorrelation function based on second order vibrational perturbation theory, with potential force fields calculated by equation of motion coupled cluster methods. Reprinted from Ref. [1] with permission of the American Chemical Society.

2.1 High-temperature chemistry in microreactors

The behavior of radicals becomes even more important and complicated in extreme environments, such as the high temperatures found in pyrolysis and combustion. To help dissect the resulting complex reaction networks into elementary steps, we use microscale flash pyrolysis reactors (“microreactors”) that achieve microsecond-scale residence times to minimize secondary chemistry by fast heating to generate radicals, followed by rapid cooling to near absolute zero.

We recently leveraged microreactor technology to study the previously unobserved role of ethyl radical in ethane pyrolysis, a fundamental chemical process of great importance in modern chemical industry [3]. The experiments were performed at the VUV beamline of the Swiss Light Source, which is also equipped with an *i*²-PEPICO spectrometer, and the combination of these three experimental elements allowed us to detect ethyl radical directly. Interpreting the data was aided greatly by the additional use of partially deuterated ethane, which produced remarkably simple

diagnostic isotopologue patterns in the mass spectra (Figure 2), and by master equation kinetics analysis based on high-level quantum chemistry calculations and computational fluid dynamics simulations. Together, these methods not only detected the last hypothesized intermediate in the reaction network for ethane decomposition but also revealed that bimolecular reactions (particularly catalytic attack of ethane by H atoms) play a vital role even under dilute conditions at short times. Accordingly, our group is developing transparent microreactors for spectroscopically monitoring radical kinetics with time-resolution significantly better than the microsecond timescales offered by post-microreactor diagnostics [4], while simultaneously applying current microreactor methods to chemical problems of environmental and energy importance [5].

2.2 Plasma chemistry

Another perhaps even more exotic regime of conditions can be found in plasmas, where reactive species and high-energy states rarely encountered even in pyrolysis are commonplace. A particularly interesting type is “cold” plasma, where incomplete thermalization (e.g. at low pressures) maintains high electron energies that can drive difficult chemical reactions without intensive power input typically lost as heat. The non-equilibrium and reactive nature of these plasmas call for non-invasive diagnostic methods that can identify reactive intermediates, quantify excited state populations,

and measure the distribution of energy between the various degrees of freedom. We have recently used a combination of simulations with optical emission spectroscopy and mass spectrometry to characterize cold plasmas with potential for environmental applications such as waste treatment and sustainable energy carrier production [6].

The extraordinary chemistry of plasmas has been leveraged to produce unusual radical and ionic species relevant for example in astrochemistry. As part of an ongoing collaboration with the McCarthy group at the Harvard-Smithsonian Center for Astrophysics and the Changala group at JILA, we are exploring novel organometallic molecules that are likely to be found in space and are also thought to have favorable properties for laser cooling and precision physics. The synthesis of such species for spectroscopic characterization involves plasmas both from laser ablation and a subsequent electric discharge in a supersonic jet source, and we are pursuing both experimental diagnostics and quantum chemical calculations to assist in optimizing the production of elusive hypermetallic molecules [7].

3. Spectroscopy

The pursuit of understanding of reactive species and their chemistry often inspires the development of novel spectroscopic methods for their detection. Examples of

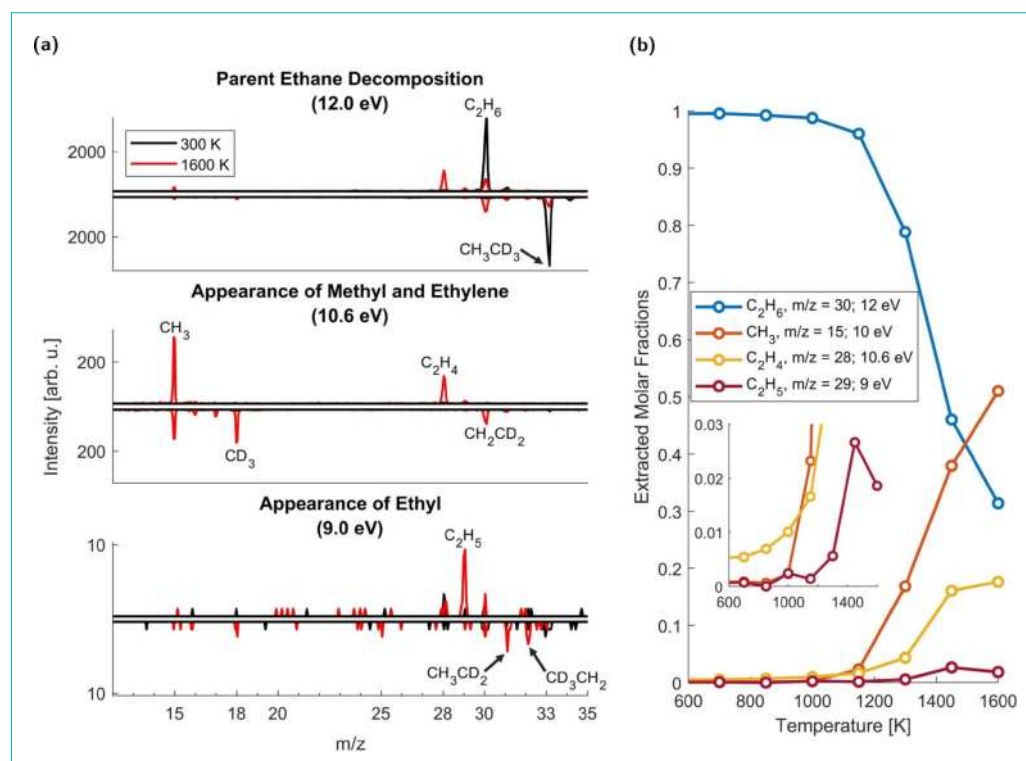


Figure 2. (a) Photoionization mass spectra of pyrolysis products of ethane and d_3 -ethane. The distinctive isotopologue patterns in the latter reveal key aspects of the mechanism. (b) Selected products as a function of temperature, showing the narrow window for detection of ethyl radical, even with the use of a flash pyrolysis microreactor. Reprinted from Ref. [3] under a CC BY-NC-ND 4.0 license.

desired improvements could include increased sensitivity, better species and even quantum state selectivity, expanded scope of applicable conditions, or ability to more accurately quantify concentrations.

3.1 Laser ionization and detection methods for molecular oxygen

The vital importance of molecular oxygen needs no introduction. Its unique properties arise from its bi-radical triplet electronic structure, which along with its ubiquity poses well-known spectroscopic challenges, e.g. spin-forbidden transitions until the eponymous vacuum ultraviolet. One specific long-standing obstacle is detection of O_2 in trace concentrations at low temperatures with quantum state resolution, such as would be desirable for investigating its reaction dynamics with radicals or at surfaces, for example; O_2 is significantly less amenable to the typically applied sensitive laser spectroscopy and mass spectrometry technique resonance-enhanced multiphoton ionization (REMPI) that is very effective for many other fundamental molecules.

REMPI of O_2 is nevertheless widely applied in studies related to environmental, combustion, and plasma monitoring, in addition to attempts to utilize it for laser ignition technology. The core challenges are the low efficiency of the process in O_2 and the need for high (deep) UV intensities at specific two-photon excitation wavelengths that are most often generated by inefficient multi-step non-linear optical processes. Furthermore, by far the strongest known transitions (near 287.5 nm via the $C\ 3s\sigma\ ^3\Pi_g$ state) suffer from significant

predissociation and even power broadening, which limit the obtainable quantum state information, the achievable sensitivity, and the effectiveness of the technique.

We recently discovered a two-color REMPI process for O_2 that is surprisingly more efficient than the simpler known one-color techniques [8] (patent pending), jointly with Prof. I. Bar (BGU). This 2+1' REMPI method (illustrated in Figure 3) utilizes more readily and economically available lower energy photons to enhance the ionization probability following UV two-photon excitation. It furthermore provides improved sensitivity and uncompromised quantum state selectivity. We have already utilized this new approach to detect vibrationally excited O_2 under ultrahigh vacuum conditions compatible with surface scattering studies in collaboration with Prof. I. Rahinov (Open University of Israel) and the Wodtke Department for Dynamics at Surfaces at the Max Planck Institute in Göttingen [9]. The potential of the method for practical applications in laser ignition is currently being explored in our laboratory.

3.2 Ultraviolet intracavity laser absorption spectroscopy

Quantitative non-invasive detection can be accomplished with absorption spectroscopy, but straightforward single pass implementations often suffer from low sensitivity. One absorption spectroscopy variant capable of detecting reactive intermediates in extreme environments is intracavity laser absorption spectroscopy (ICAS) [10]. Essentially, ICAS dramatically multiplies the effective absorption pathlength,

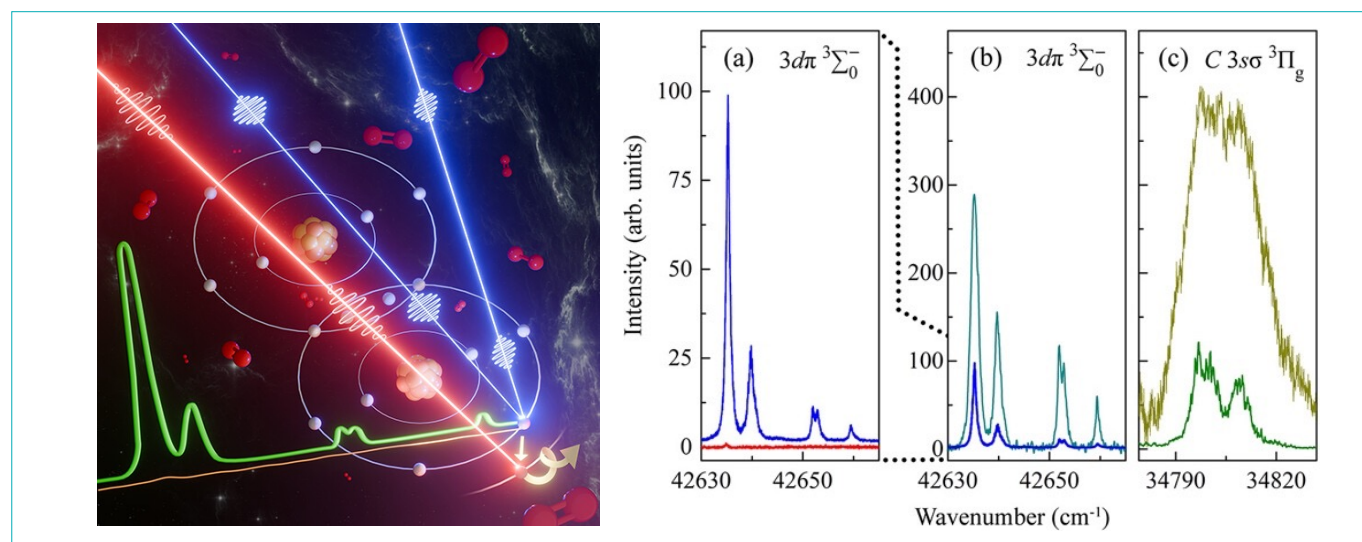


Figure 3. Two-color resonantly enhanced multiphoton ionization of molecular oxygen. (left) artistic rendering, (right) comparison of two-color REMPI spectra in blue and teal with low and medium laser pulse energy, and one-color REMPI in red (a,b); (c) One-color REMPI via the stronger but broadened 287.5 nm transition with high (green) and very high (yellow) laser power for reference. Reprinted from Ref. [8] with permission of the American Chemical Society.

and therefore the experimental sensitivity, by placing the sample inside the cavity of a broadband laser such that the light passes through the sample many times. By interacting directly with the lasing gain mechanism, the technique achieves other key relevant advantages, including multiplexed detection, immunity to broadband losses, versatile dynamic range, and the possibility for high temporal resolution. The disadvantage inherent in this operating principle is the requirement for an appropriate broadband gain medium in the wavelength range of interest. While ICAS has long been practiced in the near infrared and visible regions using well-known gain media, other spectral ranges (where laser radiation is typically generated using non-linear optical techniques incompatible with ICAS) have remained inaccessible.

We have recently extended ICAS to the vital ultraviolet spectral region (in collaboration with Prof. I. Rahinov) [10,11]. Here the strength and rich complexity of electronic transitions promise to afford many opportunities for trace detection and spectroscopic investigation of important molecular species. The key ingredient is a cerium-doped crystal gain medium such as Ce:LiCAF, which lases analogously to the well-known class of Nd-doped materials, but in the 270–320 nm range. The resulting UV-ICAS system is illustrated schematically in Figure 4 and shown in Figure 5, with a butane flame delivering a sample of hydroxyl radicals. Despite severe technical limitations in the nanosecond pulsed low repetition rate prototype, we achieved single-shot quantitative concentration and temperature measurements of hydroxyl (Figure 6), a detection limit of close to 100 ppm for sulfur dioxide, and the highest resolution absorption spectrum of

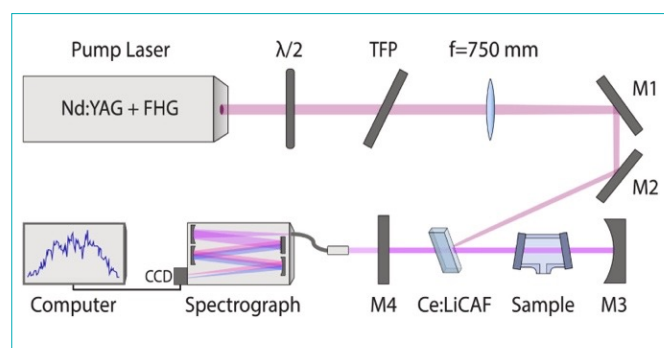


Figure 4. Ultraviolet intracavity laser absorption spectroscopy (UV-ICAS) system schematic, consisting of deep UV (266 nm) pumping of a Ce:LiCAF-based laser cavity containing the sample of interest. The absorption spectrum of the sample is then obtained by dispersing the broadband laser output in a spectrograph. 266 nm pump optics: $\lambda/2$ – half-wave plate; TFP – thin film polarizer; M1, M2 – mirrors. Laser cavity: M3 – high reflector mirror; M4 – output coupler. Reprinted from Ref. [11] with permission from Elsevier.

formaldehyde yet obtained in this wavelength region, all with significantly faster data acquisition compared to other UV absorption spectroscopy methods. We believe that this approach will offer other spectroscopic advantages as well, such as immunity to the serious challenges posed by quantum yield to many non-absorption-detection-based electronic spectroscopy methods.

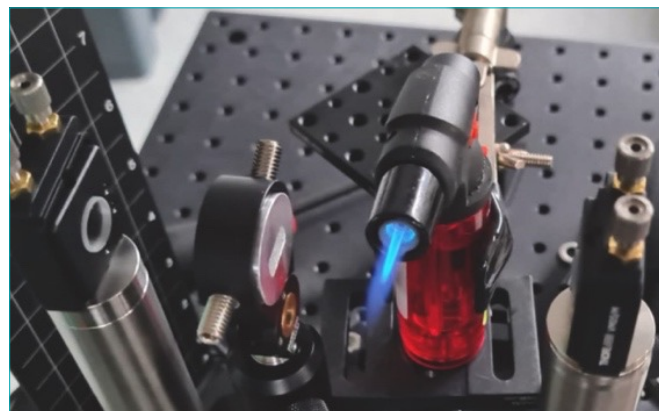


Figure 5. Photograph of a butane torch flame inside the UV-ICAS cavity to provide a sample of high-temperature hydroxyl radicals for absorption measurements (see Figure 6). From left to right: high reflector, Ce:LiCAF gain medium, torch flame, partial reflector output coupler. Reprinted from Ref. [11] with permission from Elsevier.

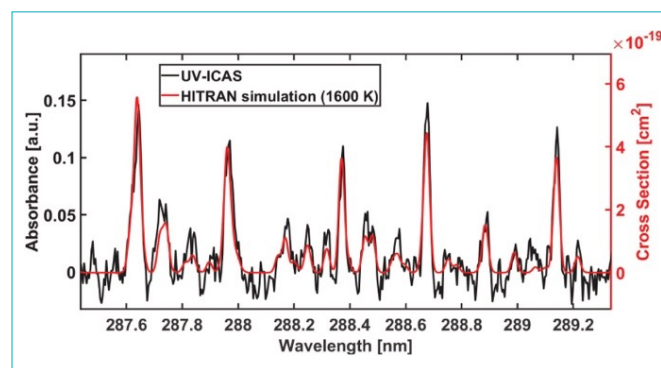


Figure 6. UV-ICAS absorption spectrum of a portion of the 1-0 electronic band system of hydroxyl radical in a butane torch flame, enabling single shot in situ temperature and quantitative concentration measurements. Reprinted from Ref. [11] with permission from Elsevier.

Ongoing continuing development of the UV-ICAS spectrometer in our group aims at dramatic improvements in resolution, sensitivity, throughput, and flexibility via a complete redesign compatible with the ultimate potential of the technique. Preliminary results are very promising.

4. Conclusions

The wide variety of fundamental and applied topics that intersect at spectroscopy of reactive molecules point to increasing importance of this research area as chemists attempt to develop ever more detailed understanding of and greater control over reactions. The growing depth and scope of these efforts will continue to drive the need for innovative approaches to characterize elusive species at the quantum state level.

Acknowledgements

I would like to thank the members of my group and our collaborators for their essential contributions to the work described above. Support from many colleagues and Ben-Gurion University of the Negev was also vital and much appreciated. Last but not least, our research has been generously funded by the European Research Council, the U.S.-Israel Binational Science Foundation, the Israel Science Foundation, the Pazy Foundation, the Israel Ministry of Energy, and the Wolfson Foundation.

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How avalanche photodiode array technology is transforming the spectroscopy of multiply excited quantum-dot emitters

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Abstract

Colloidal semiconductor nanocrystals can be very versatile sources of multiple correlated photons “on demand,” resulting from emission cascades from multiply excited states to the ground state. The study of such emission cascades at the single nano-emitter level has long been hampered by technical limitations. The advent of single-photon avalanche photodiode arrays in the last decade has dramatically simplified these measurements and significantly expanded the scope of possibilities in characterization of multiphoton emission cascades, especially in the presence of broadening, as is the case for room-temperature measurements. Some of these advances are presented here.

1. Introduction

Recent years have seen a surge of interest in sources of nonclassical light, especially in the context of applications such as quantum communication, quantum cryptography, and quantum computing, each of which has the potential for transformative change in the technological landscape. Much of the current technology relies on the process of spontaneous parametric down-conversion (SPDC) for generation of nonclassical states of light. This process involves the conversion of a single high-energy photon to two correlated low-energy photons which can be entangled. However, one of the issues with this type of source is its stochastic nature. That is, it is not possible to predict a-priori when in the photon stream SPDC will occur. As a result, special

attention has been put into the study and development of “on demand” sources of nonclassical light, where the timing can be accurately controlled. One of the promising sources of this type is based on a cascaded emission process in doubly (or higher) excited states in colloidal semiconductor nanocrystals (also known as colloidal ‘quantum dots’ (QDs)). These nanocrystals [1], the discovery of which was recognized by the Nobel Prize in Chemistry in 2023, have been extensively studied in the last three decades, and have recently become a standard component in displays and light-emitting devices, mostly as fluorescent down-converters or as active components in light-emitting diodes. Yet, their exploitation as sources of nonclassical light significantly lags behind other potential candidates, such as the related epitaxially grown semiconductor quantum dots [2]. In part, this is due to the

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difficulties in performing detailed spectroscopic studies on these inherently less stable systems.

Here, recent progress in single nanocrystal spectroscopy is described, harnessing the newly introduced single-photon sensitive avalanche photodiode (SPAD) array detectors [3]. Using these detectors, with their superb timing precision, high detection yield and large number of pixels, offers an opportunity to study with unprecedented precision emission cascades from single nanocrystals without the need to place them in a cavity or in a specific dielectric environment. As such, it dramatically increases the potential range of the spectroscopic use of emission cascades, as well as the ability to use emission cascades in sensing and imaging applications.

1.1 Colloidal semiconductor nanocrystals

Colloidal semiconductor nanocrystals [1], first introduced in the early 1980's, have rightfully been described as “artificial atoms” due to their characteristic discrete energy-level structure in the strong confinement regime. When the nanocrystal diameter is significantly smaller than the characteristic dimension of an optical excitation, the exciton Bohr radius, a regime described as “strong confinement,” the band gap of the nanocrystal deviates significantly from that of the bulk material and the absorption and emission spectra exhibit discrete excitonic transitions. In this regime, the energy-level structure can be quite well approximated by a simple “particle-in-a-box” description for noninteracting electron and hole, treating the Coulomb attraction between the two as a correction term. The characteristic emission from these discrete levels has served as the basis for the widespread use of colloidal quantum dots as tunable (relatively) narrow-band emitters in display, lighting, and bioimaging applications, especially since modern synthetic protocols allow for fabrication of quantum-dot ensembles with a narrow size distribution. Notably, however, progress in other lines of implementation, and in particular the use of colloidal quantum dots as gain media in lasers and amplifiers, has been

hampered by another aspect of their energy-level structure – the degeneracy of the energy levels, a behavior which differs significantly from the “artificial atom” description or from other luminescent materials such as organic dyes.

1.2 Multiply excited states in quantum dots

One immediate consequence of the degeneracy of energy levels is the ability to multiply excite colloidal quantum dots [4]. Since the lowest excited state is (at least) doubly degenerate, the consecutive absorption of two photons by a single quantum dot leads to the formation of state which can, in principle, emit two nearly degenerate photons whose energies are separated by the interaction energy of the two excitations in a cascaded process. The doubly excited (“biexciton”) state is typically weakly bound such that the first emitted photon is slightly red-shifted relative to the second, as demonstrated in Figure 1. Such emission cascades appear to present an excellent opportunity to generate highly tunable “on demand” photon pairs, as has been demonstrated in epitaxially grown quantum dot systems and particularly the InAs/GaAs one. Unfortunately, the emission quantum yield of the doubly excited state is typically low due to an interfering nonradiative decay mechanism termed “Auger recombination” by which one excitation in a multiply excited state recombines, but transfers its energy to one of the spectator charges remaining in the quantum dot rather than emitting it as a photon. The resultant hot carrier typically relaxes to the band edge via multiphonon relaxation within picoseconds, much faster than characteristic radiative decay times of nanoseconds. Auger recombination, which becomes more dominant as the nanocrystal size is reduced, thus renders not only exploitation of emission cascades hard, but also their spectroscopy difficult, especially at the single particle level, since Auger lifetimes become shorter than typical temporal resolutions of single-photon detectors. Therefore, historically, much of the spectroscopic work on the properties of multiply excited states (i.e. characterization of the biexciton binding energy, the Auger decay rates, and relaxation pathways of even higher excited states such as the triply excited one) have been performed at the ensemble

Daniel Amgar is a post-doctoral fellow at the Weizmann Institute. She received her MSc degree from the Hebrew University of Jerusalem, where she focused on the synthesis of perovskite nanocrystals for optoelectronic applications, and obtained her PhD from the Weizmann Institute, investigating light-matter interactions through single-particle spectroscopy. Her research focuses on optical spectroscopy of colloidal semiconductor nanocrystals and quantum-dot-based devices.



level, typically using ultrafast spectroscopy. While methods such as transient absorption, fluorescence up-conversion or multidimensional spectroscopy have indeed revealed many aspects of these multiply excited states, such as the inverse scaling of the nonradiative Auger rate with the nanocrystal volume and the dependence of the biexciton binding energy on quantum dot size and composition, there are significant limitations to the use of ensemble spectroscopic techniques. These are due to the difficulty in isolating contributions from interfering states such as the emission from charged states, and especially the inability to directly apply the findings in applications where the heterogeneity between different nanocrystals in the ensemble can be critical, such as in the use of quantum dots as sources of nonclassical light (where post-selection of suitable nanocrystals is possible).

Fortunately, the advent of detector technology has recently enabled this gap to be bridged with the introduction of SPAD arrays, exhibiting a unique combination of single photon sensitivity, high detection yields and the ability to spatially multiplex the detection.

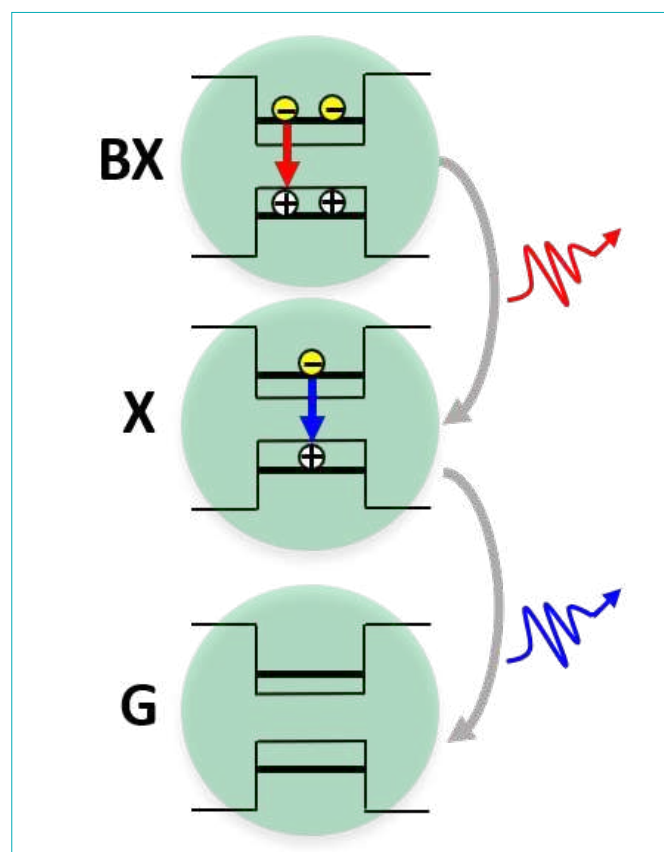


Figure 1. Cascaded emission from a doubly excited QD manifested by the emission of two sequential nearly degenerate photons. BX, X, and G stand for biexciton, exciton, and ground state, respectively.

1.3 SPAD array technology

Individual silicon-based avalanche photodiodes have been used since the early 1950's as detectors of light, and their operation parameters in Geiger mode (as single photon detectors) became more commonplace in the early 1980's, with the availability of commercial SPADs. Over time, they became the technology of choice for quantum optical applications and for time-correlated single photon counting, providing a good time resolution (well below 1 ns) at low photon fluxes and high detection quantum yields, especially in the visible and near-infrared regions. The manufacture of these, however, relied on nonstandard fabrication processes, and it is the development of complementary metal-oxide-semiconductor (CMOS)-compatible SPAD technology that dramatically expanded the possibility to design much broader classes of SPAD-based detectors and opened the pathway towards development of SPAD arrays. SPAD array technology has matured over the past decade, such that many variants and geometries of these detectors are now commercially available [3].

In the context of time-resolved spectroscopy, SPAD arrays can be divided into two categories. Smaller arrays (up to of the order of a thousand pixels) often incorporate time-to-digital converters (TDCs) for every pixel or every group of pixels, enabling direct extraction of timing information for every photon detected and functioning, for practical purposes, as “event-based” cameras, where every photon detection is logged. Larger arrays (now reaching about one megapixel) are often gated, yielding binary output frames within a certain time-gate, but not direct timing information. Dynamics can then be extracted from observing multiple frames at different gating times.

2. SPAD array based heralded spectroscopy

The fact that SPAD array detectors serve as “event based” cameras with a high time precision makes them ideal for the study of emission cascades from quantum dots. This is because the characteristic time resolution (of the order of 100 ps) is typically shorter than radiative decay in quantum dots. As such, it is simple to establish the order of events in a detected emission cascade. As SPAD arrays have versatile configurations, they can simultaneously perform measurements in additional dimensions (space, frequency, spatial frequency, polarization, as long as these dimensions can be spatially mapped onto the SPAD array), while maintaining the time resolution, thus enabling spectroscopic characterization of individual emission cascades from a single quantum emitter, as described below in sections 2.1 and 2.2. This type of measurement is very simple to perform and only requires a microscope equipped with a high numerical

aperture objective to efficiently collect emitted photons. The critical point is that the use of a SPAD array detector allows to post-select from the stream of collected photon detection events only those which fit the profile of the event under study (for example a pair of photons emitted from a biexciton-exciton cascade), and the order of arrival of photons within that event is clearly set from the timing information [5]. The ability to perform this depends critically on the detection efficiency. The collection efficiency of a free-space objective is about 30%, and the detection yield of SPAD arrays is currently capped at about 50%. Considering additional loss channels, the overall detection efficiency is of the order of 10%, corresponding to 1% probability of detection for photon-pair events and 0.1% for photon triplets. These values set the limit of detectability of emission cascades, dictating that photon pair events can be quite readily measured even for dim nanocrystals (biexciton quantum yield of 1% or so and a reasonable quantum yield for the singly excited state), but measurement of triplets requires very bright particles [6].

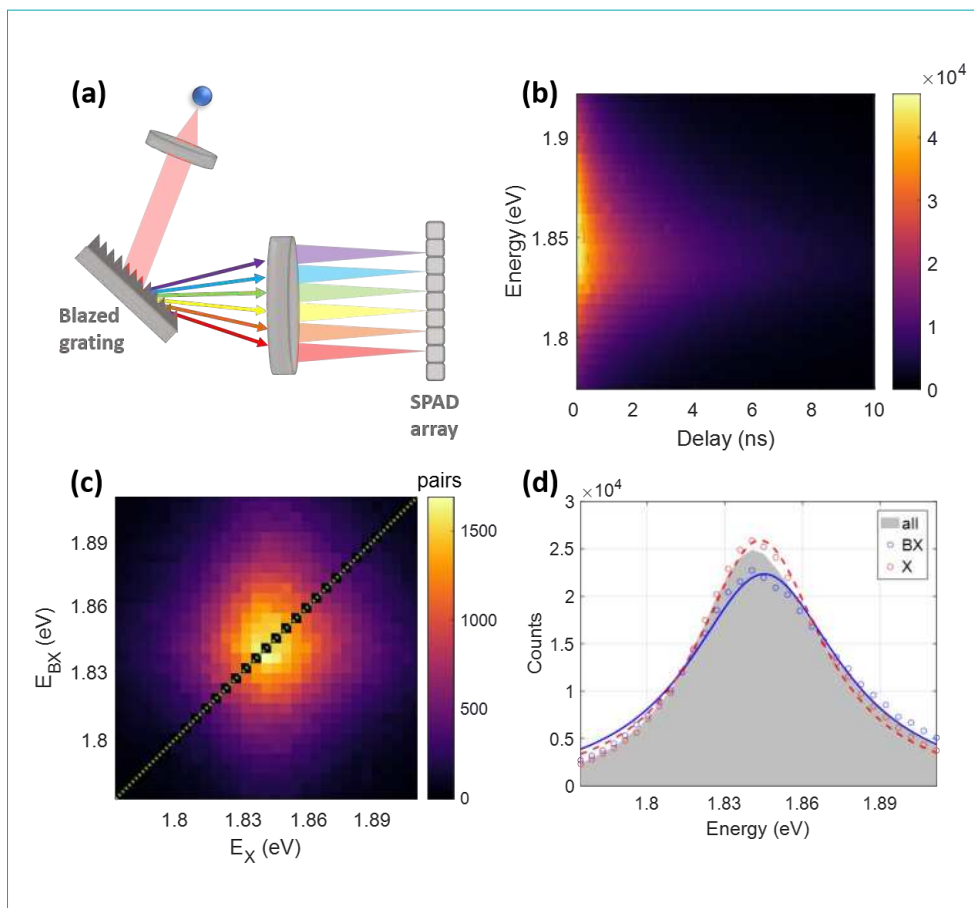
As examples of heralded spectroscopy, the following subsections describe mapping out of multiexciton energetics

by heralded spectroscopy in the frequency domain, and study of the biexciton dipole moment by spectroscopy in the spatial frequency domain.

2.1 Elucidating the energetics of multiply excited states

The first implementation of heralded spectroscopy utilized a linear SPAD array in a spectrometer configuration, as described in Figure 2a. In this setting, the wavelength of every photon is mapped to the pixel number in a linear array while arrival times enable differentiation between the first and second arriving photons in a biexciton-exciton-ground state cascade [5,7]. Figure 2b demonstrates an energy-time histogram that can be obtained from a typical single-particle measurement. When studying the doubly excited biexciton state, care must be taken to excite the quantum dot well below saturation such that the probability of exciting the triply excited state is negligible. For higher states, it is reasonable to work around the saturation level of $\langle N \rangle \sim 1$ absorbed photon per pulse per dot. This type of measurement provides direct access to several key spectroscopic properties. In the case of the doubly excited state, the arrival times of all first

Figure 2. Heralded spectroscopy implemented by a linear SPAD array. (a) A scheme of the single-photon spectrometer coupled to the linear SPAD array detector. The photoluminescence from a single QD is imaged onto the pixel array such that the arrival time and color of each detected photon can be resolved. (b) A two-dimensional histogram of parallel time and spectrum detection obtained from a typical single-particle (nanoplatelet) measurement. (c) A two-dimensional histogram of photon pairs detected within the same excitation cycle showing the energy of the first arriving photon (biexciton) and the energy of the second arriving photon (exciton). The dashed green diagonal serves as a guide to the eye and marks the same energy for both photons. (d) Spectra of the biexciton (blue circles), exciton (red circles), and all on state detections (gray area, normalized). Solid blue and dashed red lines are fits of the biexciton and exciton spectra, respectively, to a Cauchy-Lorentz distribution.



arriving photons can be histogrammed, providing access to the (typically nonradiative, determined by the Auger rate) decay rate of the biexciton state. Similarly, the histogram of the delay times between the arrival of the first and second photons reveals the (usually radiative decay dominated) decay rate of the singly excited state. Finally, as the energy of both photons is measured, a two-dimensional histogram of one versus the other can be drawn, as shown in Figure 2c. Every nanocrystal is characterized by a roughly circular blob in such a plot, where the diameter is given by the emission linewidth. The distance of the center-of-mass of the blob from the diagonal represents the biexciton binding energy, a quantity which, at room temperature (where emission lines are significantly broadened), was previously measured only at the ensemble level. Notably, this type of analysis can also be readily applied to triply excited states if the emission quantum yield of the highly excited states is sufficiently high (as often occurs for nanocrystals in the intermediate to weak confinement regime). By full horizontal and vertical binning of Figure 2c, one can directly plot the biexciton and exciton spectra, respectively, as presented in Figure 2d, and reveal the biexciton binding energy from the energy difference of the biexciton and exciton spectral peaks.

A key advantage of heralded spectroscopy is the natural post-selection of emission events arising from the desired state. Ensemble spectroscopy is often plagued by contributions from undesired states such as trions (charged excitons). These do not contribute, however, to photon-pair detection. Importantly, the criteria for post-selection of emission cascades can be tailored to the particular problem, providing significant versatility.

2.2 Elucidating the dipole moment of multiply excited states

Another realization of heralded spectroscopy utilizes defocused imaging to characterize the differences in emission dipole moment between the lowest emitting state and a higher emitting state [8]. Defocused imaging maps the emitter orientation onto a 2D image of spatial frequencies at the detector, as shown in Figure 3. Similar to heralded spectroscopy, each pixel (now in a two-dimensional array) corresponds to a range of spatial frequencies, and by post-selecting pairs of photons emitted following a single excitation pulse, the dipole emission pattern of higher excited states such as the biexciton state can be resolved.

Figures 4a,b exemplify the result of a typical measurement of a single elongated nanocrystal, utilizing heralded post-selection of photon pairs to isolate the dipole emission of the biexciton state from that of the single exciton state. The polar plots of each excited state were extracted by fitting the number of photons detected by the central six pixels of the detector

(marked with blue circles in Figure 3ii), which contain most of the anisotropic emission information, to a sum of a squared sine and an isotropic background. This enables the extraction of, most importantly, the emission anisotropy, but also the orientation of the nanocrystal. By clustering the anisotropy values, it is possible to probe very weak effects on the dipole emission pattern of the biexciton. Figure 4c displays the anisotropy values of tens of single nanorods from the same sample, showing a weak but statistically significant difference in the emission anisotropy between the exciton and biexciton. Unlike the electrostatic interaction between two excitons,

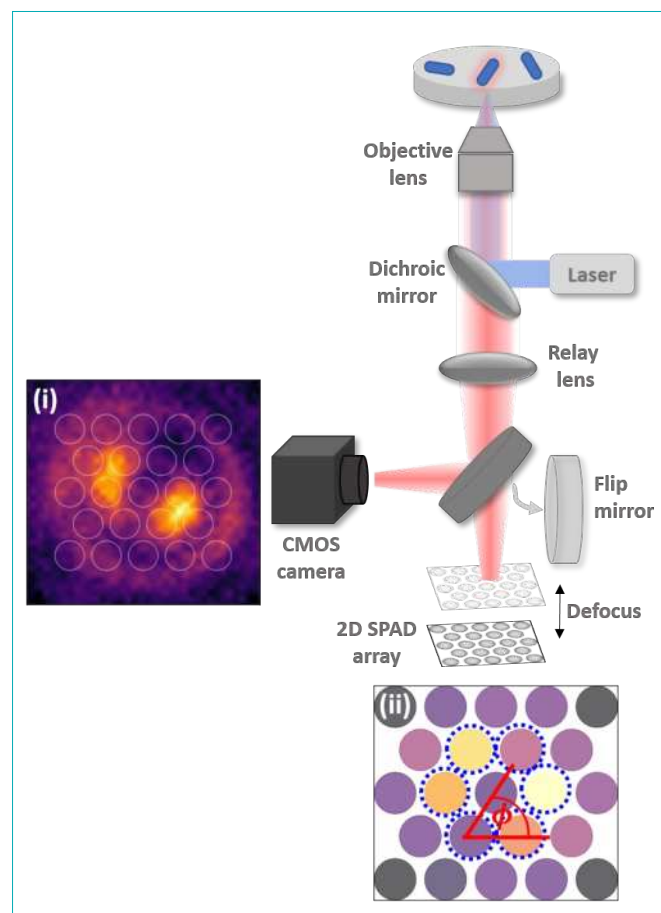


Figure 3. Defocused imaging integrating a two-dimensional SPAD array for the characterization of the transition dipole moment of an anisotropic nanocrystal. The defocused dipole emission pattern from a single nanorod is imaged onto a SPAD array and can be time-resolved to explore higher excited states emission anisotropy. (i) Defocused image of a single nanorod imaged with a CMOS camera. The overlaid white circles represent the area collected by the pixels of the SPAD array detector. (ii) Analyzed SPAD image which shows the histogram, by pixel, of all detected photons. The angle θ (in red) visualizes the in-plane orientation of the measured nanorod according to the intensity distribution. Insets (i) and (ii) are adapted with permission from [8] © American Chemical Society.

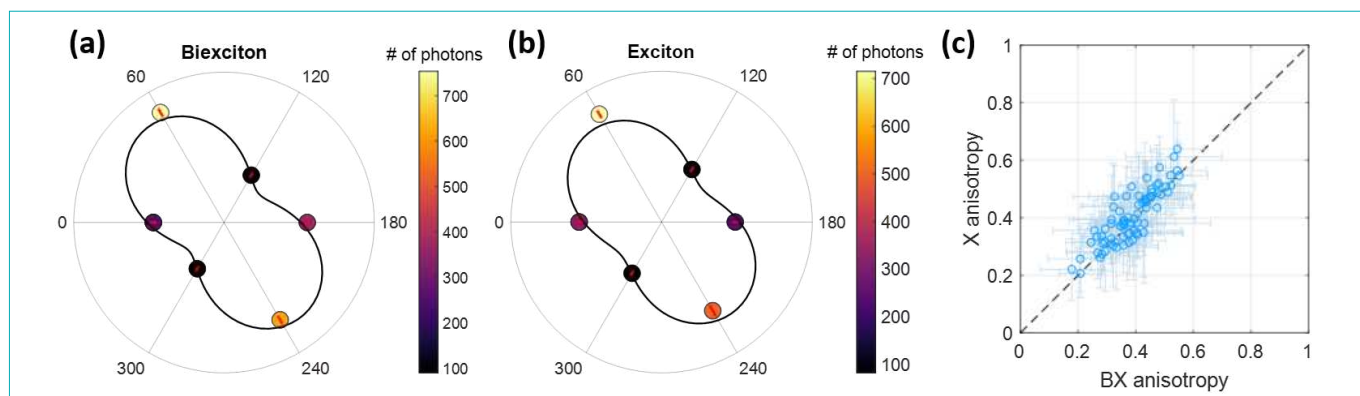


Figure 4. Heralded defocused imaging. Polar representation of the intensity values recorded by the six pixels of the SPAD array (marked by blue circles in Figure 3) for the biexciton (a) and exciton (b) along with the fit (black solid line) to the integrated dipole emission model. (c) Aggregate analysis of the exciton (X) and biexciton (BX) anisotropy for 79 single nanorods. The dashed black diagonal serves as a guide to the eye, indicating the same anisotropy values for both exciton and biexciton photons. Adapted with permission from [8] © American Chemical Society.

which is easily explained and comprises the major part of the spectral shift of higher excited states, effects leading to changes in the emission dipole pattern are more subtle. They include two main contributions: the first arises from the symmetry of the fine structure of excitonic states, which can differ between the singly and doubly excited states, and the second is related to transient changes in the refractive index of the material that may alter the anisotropy of the doubly excited state. The second occurs in anisotropically shaped nanostructures and relates to global changes in the dielectric constant of the nanocrystal upon photoexcitation (the reduced oscillator strength of the excitonic transition modifies the refractive index due to Kramers-Kronig relationships). Since the formation of oriented ensembles is highly impractical, heralded single nanocrystal spectroscopy appears to be the only practical method by which these effects can be measured.

3. Massively parallel spectroscopy with large format SPAD arrays

New opportunities are also becoming available with the dramatic improvement in performance of large format SPAD arrays. These are typically operated in a gated mode, and as such are incompatible with heralded spectroscopy, as they do not provide timing information for every detected photon. Yet, the sheer size enables tasks to be performed which deviate significantly from the common spectroscopy mode of one single particle at a time, as described, for example, in the above section. One example for this is the characterization of the second-order photon correlation function $g^{(2)}$ (a parameter closely related to the quantum yield of the doubly excited state) in a wide field of view, potentially enabling simultaneous measurement of thousands of particles, and paving the way to obtain statistics which far exceed those

reported in conventional single nanocrystal studies (typically tens to a few hundreds of QDs at most) [9].

Such wide-field detection of $g^{(2)}$ has been recently reported using a 0.25 megapixel SPAD array. The key operation parameter is to excite the sample using short pulsed excitation (typically around 1 ps, much less than any characteristic decay rate of the probed system) at a rate equal to the readout rate of binary frames from the detector, such that for every frame every nanocrystal is excited only by one short pulse. $g^{(2)}$ information is then extracted by imaging every nanocrystal to a small subarray of pixels (2 x 2 or 3 x 3) and analyzing near-neighbor correlations in the emission stream. An example of such a measurement is shown in Figure 5, where the intensity from a field of view where QDs have been dispersed is shown (Figure 5a), whereas the corresponding estimated $g^{(2)}$ trace is plotted (Figure 5b). While still rudimentary due to various technical issues (low collection efficiency in the absence of microlens arrays, artifacts due to the presence of “hot” pixels for which dark counts dominate the signal, etc.) they exemplify the capabilities of such an imaging apparatus.

The main difficulty in these measurements is the relatively low readout rate of current large format SPAD array detectors, typically around 100 KHz and with record rates approaching 1 MHz. This is to be compared with the 20 ns typical dead time of SPAD following detection, corresponding to a maximal achievable rate of 50 MHz. The main hurdle here involves data handling, since the data volumes from megapixel binary frames at MHz rates are already approaching the capabilities of current data transfer buses. A future solution to this issue, which is currently being studied in several laboratories worldwide, is the use of on-chip data preprocessing which can dramatically reduce the data volumes.

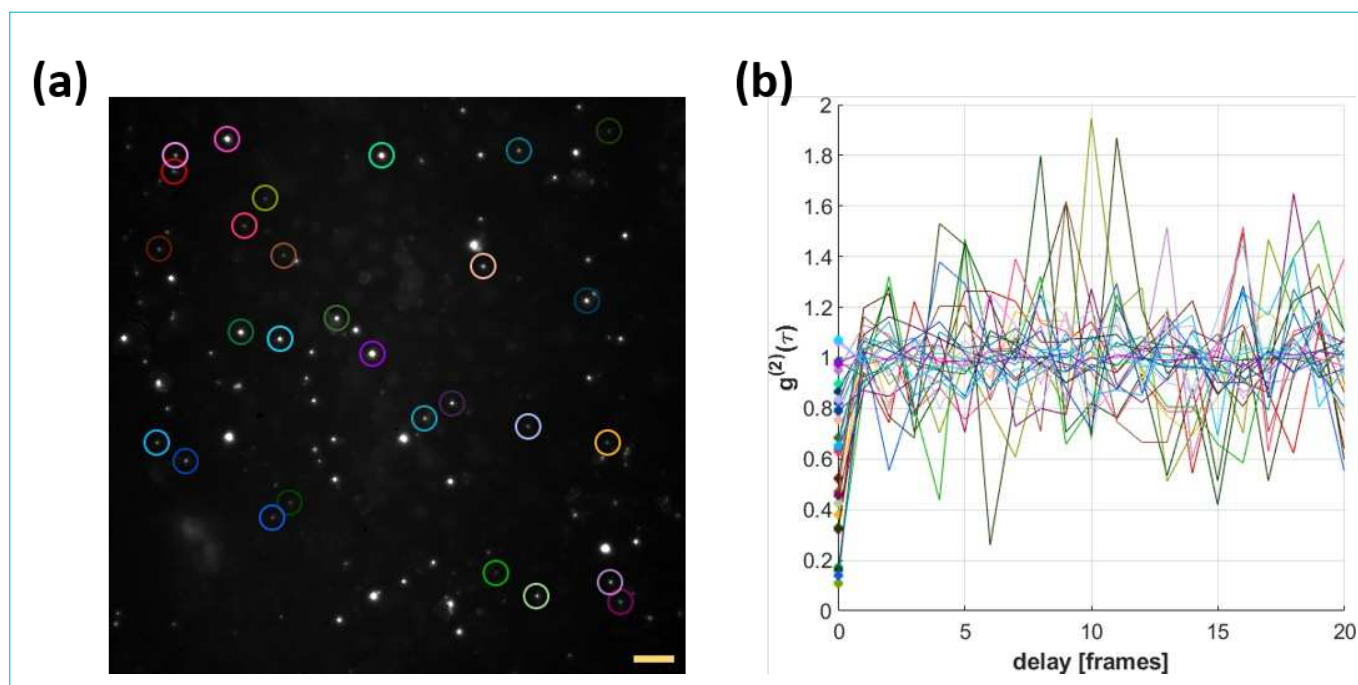


Figure 5. Intensity map and photon statistics of QDs at selected locations. (a) Integrated intensity image across the entire detector (scale bar is 5 μm). (b) Traces for representative points marked by colored circles in the intensity map. Reprinted with permission from [9] © Optica Publishing Group.

4. Conclusions

Not too long ago, even simple quantum optics measurements such as the characterization of photon statistics required strong infrastructure in the operation of delicate equipment such as custom detectors, correlation hardware and dedicated software and electronics. The advent of SPAD array technology has the potential of completely transforming this field, enabling the rapid construction of quantum optics setups and their efficient use for the spectroscopy of single quantum emitters. Colloidal QDs are a prime example of a system for which these detectors have been instrumental in revealing previously inaccessible spectroscopic information with potential application in a variety of quantum optics and spectroscopy applications.

SPAD array hardware is improving rapidly in all aspects: timing accuracy, dark count and interpixel crosstalk rates, pixel number, fill factors and spectral responsivity. The current trend of moving towards more on-chip analysis capabilities is certain to introduce many more spectroscopy options to harness this very powerful hardware for performing rapid spectroscopy on large ensembles, which can have important implications for both QD synthesis and device fabrication.

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Stochastic estimators in electronic structure theory

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Abstract

Stochastic methods offer a simple way to study chemical and material systems that are too large for conventional electronic-structure calculations. Instead of computing all quantities exactly, key physical properties are estimated by averaging over random samples. While individual samples are noisy, their average converges reliably to the correct result. We illustrate this idea using a familiar example from environmental monitoring, where correlations between pollutants can be extracted from large data streams without storing the full dataset, and then turn to a case study from quantum materials: warm dense hydrogen. In this regime, high density keeps the system strongly quantum even at elevated temperatures, placing it at the boundary between condensed matter and plasma physics. These conditions are central to planetary interiors and inertial confinement fusion and provide a demanding test for computational methods. Using stochastic density functional theory combined with Langevin molecular dynamics, we compute thermodynamic and transport properties under extreme conditions. Despite the presence of noise, equilibrium properties such as temperature and pressure are well behaved, and the electrical conductivity converges with increasing system size. By treating randomness as a computational resource rather than a drawback, stochastic estimators enable simulations of size and complexity that are otherwise inaccessible, opening new opportunities for studying realistic materials under extreme conditions.

1. Introduction

Quantum chemistry and electronic structure theory are the primary computational tools for understanding the quantum structure of matter [1-4]. While these methods excel for small molecules and idealized crystalline systems, materials science presents a fundamental challenge: complexity. Real-world phenomena rarely occur in perfect, infinite lattices; instead, they arise from disorder, interfaces, defects, and large-scale fluctuations. To understand the conductivity of a doped semiconductor junction, the catalytic activity of a

nanoparticle surface, or the equation of state of warm dense matter, one must simulate supercells containing thousands, or even tens of thousands, of electrons.

It is here that we encounter a fundamental barrier. Deterministic approaches—whether Density Functional Theory (DFT), Many-Body Perturbation Theory (GW), or linear response theory—inevitably hit a severe “scaling wall.” As the system size (N) grows, the computational cost scales as $O(N^3)$ or even $O(N^4)$, rendering these essential large-scale simulations prohibitively expensive. To bridge the gap

Roi Baer is a Professor of Theoretical Chemistry at the Institute of Chemistry, The Hebrew University of Jerusalem, where he holds the Ratner Family Chair in Chemistry. He is the Director of the Fritz Haber Research Center for Molecular Dynamics, a leading international hub for theoretical and computational chemical physics. His research focuses on developing quantum-mechanical methods for electronic structure and dynamics, with particular emphasis on density functional theory (DFT and TDDFT), open quantum-system dynamics, and stochastic approaches that overcome traditional scaling limits in quantum chemistry.

Baer is widely recognized for seminal contributions to long-range-corrected and tuned range-separated density functionals, reliable prediction of charge-transfer excitations, and the formulation of stochastic Kohn–Sham DFT, stochastic GW, and Bethe–Salpeter methods. These innovations enable accurate simulations of large molecular systems, nanostructures, and condensed-phase materials on modern high-performance computing platforms. His work bridges chemistry and physics and addresses problems ranging from spectroscopy and photophysics to quasiparticle excitations and energy transport.

He received his PhD from the Hebrew University of Jerusalem and completed postdoctoral research at the University of California, Berkeley. Baer has held visiting positions at UC Berkeley, UCLA, and the University of Southern California. His honors include the Israel Chemistry Society Prize for Outstanding Scientist, the Klachky Prize, and the Rector’s Prize for Excellence in Research and Teaching. In 2025, he joined the board of the World Association of Theoretical and Computational Chemists (WATOC).



between microscopic equations and macroscopic reality, we must rethink the very way we interrogate quantum systems.

The solution lies not in faster processors, but in a conceptual shift from deterministic calculation to stochastic sampling. In a stochastic approach, we do not attempt to compute a quantity exactly in one massive step. Instead, we estimate the quantity by drawing random samples from a carefully chosen process. First, we identify the physical quantity we need. Next, we design a random process that produces samples carrying that information. Finally, we apply a statistical rule that combines these samples into a single estimate. As we gather more samples, the estimate becomes steadily more reliable, with the average error shrinking toward zero. To illustrate this, consider an environmental agency monitoring a river. Using a Time-of-Flight Mass Spectrometer (TOF-MS), the agency generates a chemical spectrum every millisecond, producing a dataset of billions of samples (N) over a year. The agency's objective is to pinpoint pollution sources by

identifying correlations: do specific chemicals appear and disappear in unison? If the concentrations of Lead and Benzene rise and fall together, they likely originate from a common discharge pipe. Mathematically, this relationship is captured by the covariance. Suppose the stream of TOF measurements for Lead is $L=(L_1, L_2, \dots)$ and for Benzene is $B=(B_1, B_2, \dots)$. The correlation is the dot-product:

$$q = \mathbf{L} \cdot \mathbf{B} = L_1 B_1 + L_2 B_2 + \dots \quad (1)$$

To find it, one must multiply the signal intensity of one chemical by the other at every single time step and sum the results over the year. However, a brute-force analysis is practically impossible. Storing the full history of every spectrum to compute these pairwise covariances would require petabytes of memory, far exceeding available resources. The solution is on-the-fly stochastic compression.

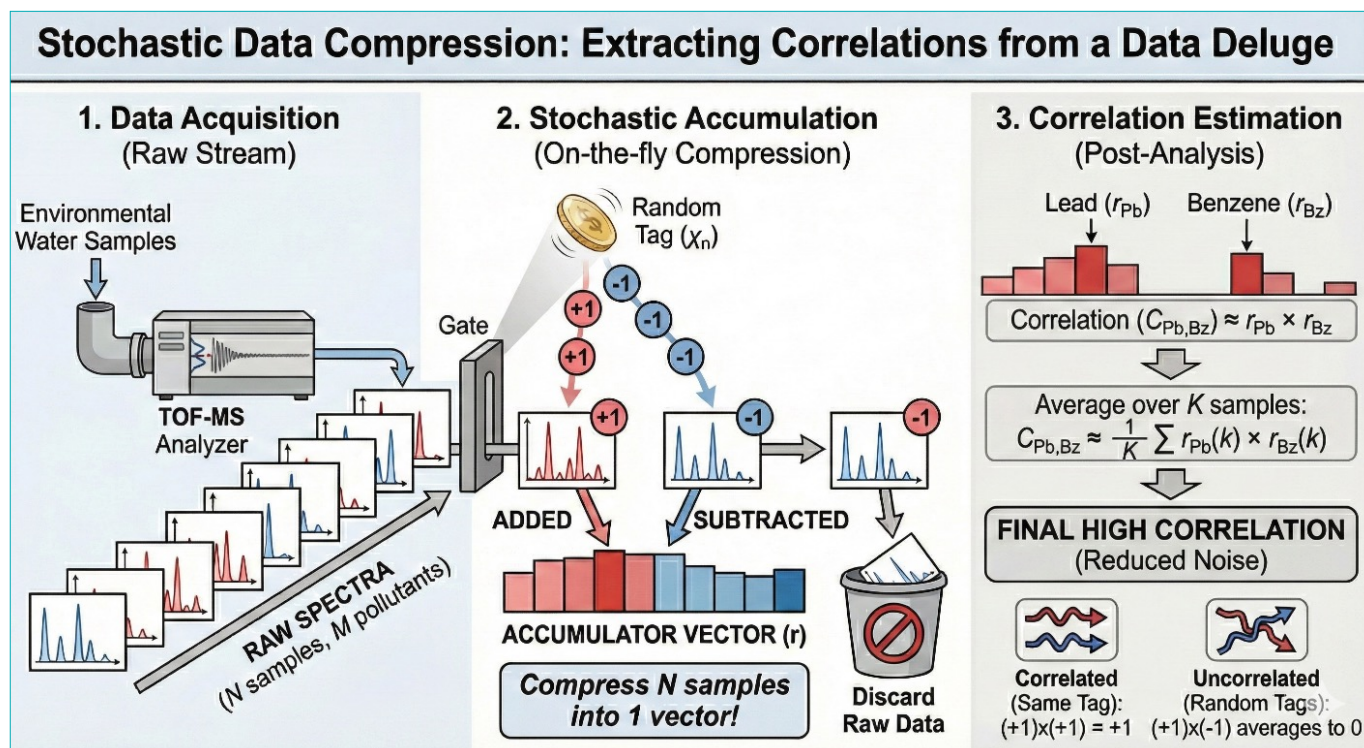


Figure 1. Stochastic compression of a chemical analysis data deluge. **Left:** Data acquisition. A high-throughput instrument (TOF-MS) generates a continuous stream of raw data vectors (spectra), representing a massive dataset of N samples that is too large to store. **Middle:** On-the-fly compression. To control statistical error, the stream is compressed into K (with K orders of magnitude smaller than N usually on the order of 10 to 100) independent vectors. For each of the K realizations, every incoming vector is assigned a random sign, ± 1 , and added to the corresponding running accumulation vectors $r^{(k)}$. **Right:** Correlation recovery. The correlation (covariance) between two features (e.g., Lead and Benzene) is estimated by multiplying their values in the compressed vectors and averaging the result over the K samples. The averaging reduces statistical noise in proportion to $1/\sqrt{K}$.

Here is the trick. We don't store the raw data. Instead, we maintain a few small "accumulation buckets." As each measurement arrives, we add it to the bucket, but we multiply it by a random coin flip ($\chi = \pm 1$). At the end of the year, we have a "compressed" vector \mathbf{r} for each chemical:

$$\mathbf{r}_{\text{lead}} = L_1\chi_1 + L_2\chi_2 + \dots \quad \text{and} \quad \mathbf{r}_{\text{benzene}} = B_1\chi_1 + B_2\chi_2 + \dots \quad (2)$$

These compressed vectors look like random noise. However, they miraculously encode the correlation of the entire year. To get the answer, we simply multiply the compressed values:

$$\hat{q} := \mathbf{r}_{\text{lead}} \mathbf{r}_{\text{benzene}} \quad (3)$$

The expected value of this simple product is exactly the true correlation: $q = \mathbb{E}\hat{q}$ where \mathbb{E} is the symbol designating expectation value of a random variable.

Why does this work? If we expand the multiplication, we see the mechanics of cancellation at play. Using the definition of \mathbf{r} , we have:

$$\hat{q} = L_1B_1\chi_1^2 + L_1B_2\chi_1\chi_2 + L_2B_1\chi_2\chi_1 + L_2B_2\chi_2^2 + \dots$$

Since our coin flips χ are always ± 1 , the squared terms are always 1 ($\mathbb{E}\chi_1^2 = \mathbb{E}\chi_2^2 = 1$).

These are the signals we want. However, the cross-terms ($\chi_1\chi_2$) are random—sometimes positive, sometimes negative—so on average, they cancel out to zero ($\mathbb{E}[\chi_1\chi_2] = 0$). We are left only with the matching terms:

$$\mathbb{E}\hat{q} = L_1B_1 + L_2B_2 + \dots$$

This matches our target equation exactly. By accepting a little bit of random noise (which we can average out), we solve a problem that was previously impossible to calculate.

Crucially, this is not just a trick for data compression; it is the same mathematical process that drives the stochastic approach to electronic structure.

2. From data streams to quantum materials

The fundamental framework for describing materials is Density Functional Theory (DFT), where the complex many-electron problem is mapped onto a system of non-interacting electrons at temperature T , governed by the Kohn–Sham Hamiltonian [5]:

$$\hat{h}_{KS} = -\frac{\hbar^2}{2me} \nabla^2 + v_{KS}(\mathbf{r}; \mathbf{R}).$$

The first term is the kinetic energy operator, and the second is the Kohn–Sham potential V_{ks} , which depends on the

electronic position \mathbf{r} and the nuclear positions \mathbf{R} . The space available to the electrons is typically infinite in extent. In practice, however, a computer cannot represent an infinite object and must work with a finite description of the electronic state. One natural way to do this is to introduce an equally spaced mesh of points spanning the simulation cell, and to represent the electronic wave functions only through their values on this grid. This is known as a grid representation. Although the number of grid points is finite, it is typically very large (on the order of millions).

The eigenvalues (energy levels) ϵ_n and the corresponding eigenfunctions ψ_n of \hat{h}_{ks} are populated according to the Fermi–Dirac distribution:

$$F(\epsilon_n) = \frac{1}{1 + e^{\frac{\epsilon_n - \mu}{k_B T}}}$$

where k_B is Boltzmann's constant. At zero temperature, only the lowest N_e levels are populated. However, at positive temperatures, essentially all N_{states} in the system are populated.

The computational bottleneck arises when calculating physical observables, such as the electron density or the electrical conductivity. In the standard "deterministic" approach, the observable is obtained by summing the contribution of every populated energy level,

$$A = \sum_{n=1}^{N_{\text{states}}} F(\epsilon_n) \langle \psi_n | \hat{A} | \psi_n \rangle,$$

where \hat{A} is the operator associated with the observable and the Dirac bra–ket denotes the integral

$$\langle \psi_n | \hat{A} | \psi_n \rangle = \iiint \psi_n^*(\mathbf{r}) \hat{A} \psi_n(\mathbf{r}) d\mathbf{r}.$$

When a grid representation is used, these integrals become very large discrete sums. In particular, the electron density at every grid point is given by

$$n(\mathbf{r}) = \sum_{n=1}^{N_{\text{states}}} F(\epsilon_n) |\psi_n(\mathbf{r})|^2.$$

In all such cases, the only way to obtain the desired quantities is to compute essentially all eigenvalues and eigenfunctions of the Kohn–Sham Hamiltonian, a task that constitutes a major computational challenge.

To bypass this massive computational effort, we introduce a stochastic approach. We define a function $\chi(\mathbf{r})$ composed of random ± 1 values on the grid, and construct a stochastic orbital

$$\phi(\mathbf{r}) := \sqrt{F(\hat{h}_{KS})} \chi(\mathbf{r}).$$

The calculation of ϕ is the primary numerical task in this approach, analogous to the time-of-flight spectrum measurement in our river analogy. In practice, it is carried out by expanding the Fermi–Dirac function in Chebyshev polynomials of \hat{h}_{KS} , thereby avoiding explicit diagonalization.

We can now define a single-shot estimator for the electron density,

$$\hat{n}(\mathbf{r}) = |\phi(\mathbf{r})|^2.$$

The physical density is obtained as the expectation value of this estimator,

$$n(\mathbf{r}) = \mathbb{E} \hat{n}(\mathbf{r})$$

without reference to individual eigenstates. Similarly, for any observable \hat{A} , the single-shot estimator is

$$\hat{A} = \langle \phi | \hat{A} | \phi \rangle,$$

and the corresponding physical value is $A = \mathbb{E} \hat{A}$.

Finally, by drawing K independent stochastic samples and averaging them, the statistical error is reduced by a factor of $1/\sqrt{K}$. This shift from deterministic summation over eigenstates to statistical averaging over random estimators constitutes the essence of stochastic density functional theory (sDFT) [6-12].

3. Langevin Dynamics and the Equation of State

The above approach allows the estimation of the force on a nucleus (at position x). However, this force estimation has the drawback that it contains random fluctuations. As a result, any deterministic molecular dynamics trajectory is going to be wrong already in its first time step. Does that mean the force is useless? That depends on what you are going to do with it.

If the goal is to predict the precise trajectory of a specific chemical reaction (e.g., a specific bond-breaking event in real time), the noise is indeed problematic. However, if the goal is to determine equilibrium properties—such as the Equation of State (EOS), structural correlation functions, or

thermodynamic averages—we can turn this drawback into a feature using Langevin dynamics.

Consider a single nucleus with mass moving in one dimension with velocity v . In standard Langevin dynamics, its motion is described by modifying Newton's equations to include a friction term and a random noise term:

$$m\dot{v} = f_{det}(x) - \gamma mv + \eta(t),$$

where f_{det} is the deterministic force when the nuclear configuration is x , γ is a friction coefficient, and $\chi(t)$ is a “white noise” term. In conventional simulations, one calculates and adds an artificial noise η to simulate a thermal bath. The magnitude of this noise is strictly tied to the friction and the target temperature T via the Fluctuation-Dissipation Theorem:

$$\langle \eta(t)\eta(t') \rangle = 2\gamma M k_B T \delta(t - t').$$

In our stochastic approach, the force estimate \hat{f} , naturally contains a random component:

$\hat{f} = f_{det} + \delta f_{fluct}$. Instead of adding artificial noise, we treat the inherent algorithmic noise δf_{fluct} as the thermal bath itself. By identifying the statistical variance of our force, we can tune the friction coefficient γ to dissipate exactly the amount of energy the noise injects.

Langevin molecular dynamics provides a controlled way to sample thermal equilibrium. Although the individual trajectories are stochastic and do not follow Newtonian mechanics, the probability of visiting a given atomic configuration follows the Boltzmann distribution exactly. As a result, thermodynamic quantities extracted from these simulations, such as the pressure and equation of state, are statistically exact despite the presence of noise at the level of individual trajectories.

4. Case study: Warm dense hydrogen

Hydrogen under extreme conditions provides a natural and widely studied test case for electronic-structure methods. At high densities and temperatures—conditions commonly referred to as *warm dense hydrogen*—hydrogen lies in an intermediate regime between condensed matter and plasma physics. In this regime, neither simple molecular models nor ideal plasma descriptions are adequate: electronic, ionic, and thermal effects are all strongly coupled.

Interest in dense hydrogen dates back to the classic work of Wigner and Huntington, who predicted that hydrogen would undergo pressure-induced metallization. Today, warm

dense hydrogen plays a central role in planetary science, where it governs the internal structure and magnetic fields of giant planets, and in inertial confinement fusion, where hydrogen isotopes are driven to extreme states by laser compression. Accurate predictions of thermodynamic and

the number of electrons is kept fixed at $N_e=128$ by adjusting the electronic chemical potential at each time step. In the μVT simulation (right), the chemical potential is held fixed and the number of electrons is allowed to fluctuate.

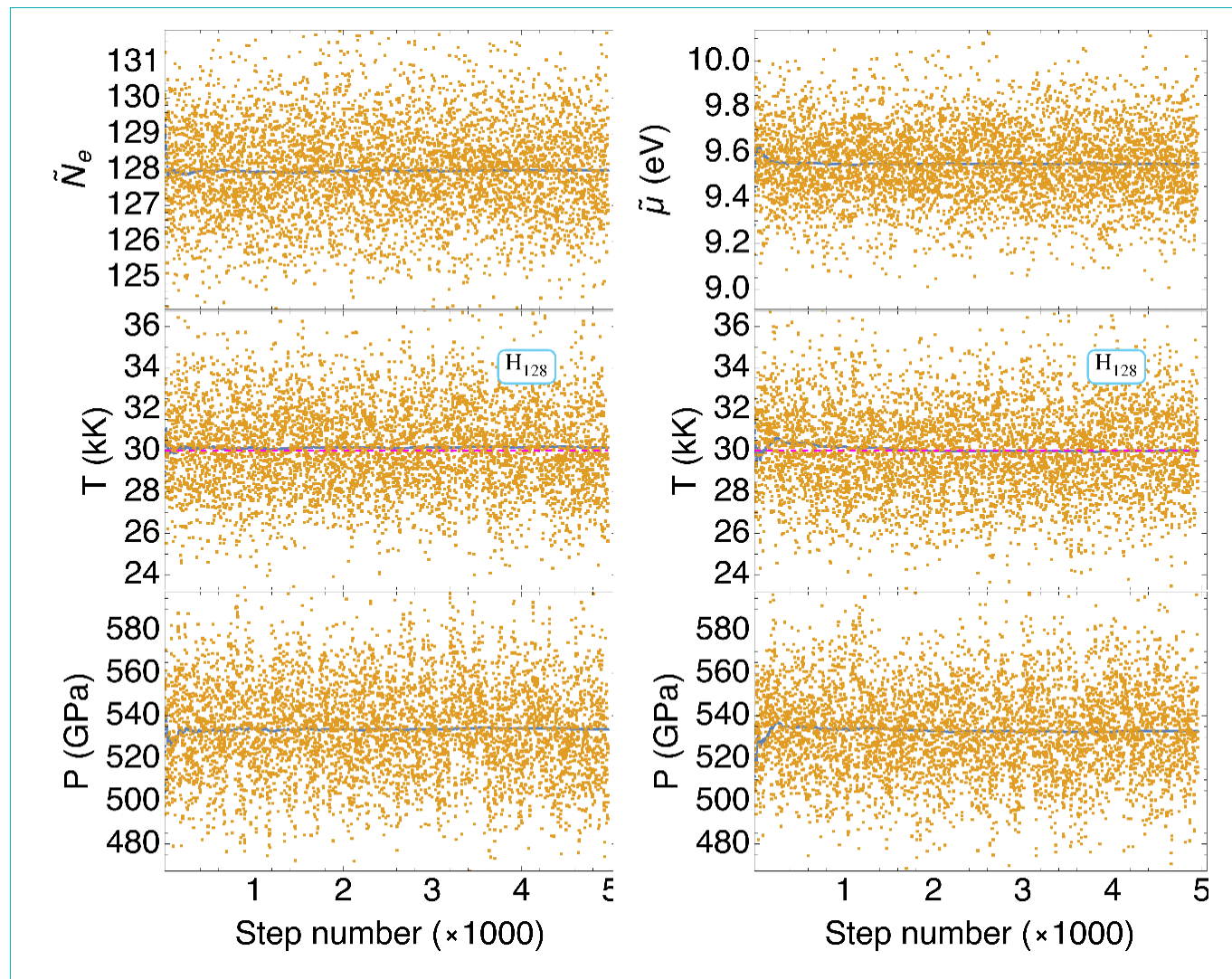


Figure 2. Time evolution of selected quantities in two Langevin molecular-dynamics simulations of Hydrogen. Brown points show instantaneous values and blue curves show running averages. In the left panel, the number of electrons is fixed by adjusting the chemical potential at each time step. In the right panel, the chemical potential is fixed and the number of electrons is allowed to fluctuate. In both cases, temperature and pressure remain stable, indicating well-equilibrated dynamics.

transport properties in this regime remain challenging, both experimentally and computationally, making it an ideal setting for testing stochastic approaches.

Figure 2 illustrates this behavior by comparing two Langevin trajectories of hydrogen computed in different electronic ensembles. (See Footnote 1). In the $N_e VT$ simulation (left),

In both cases, the system remains well equilibrated. The kinetic temperature—measured from the average nuclear kinetic energy—stays closely centered around the target value, and the pressure fluctuates around a stable mean. While the chemical potential fluctuates in the μVT ensemble and the electron number fluctuates in the ensemble, their time-averaged values closely match the corresponding fixed

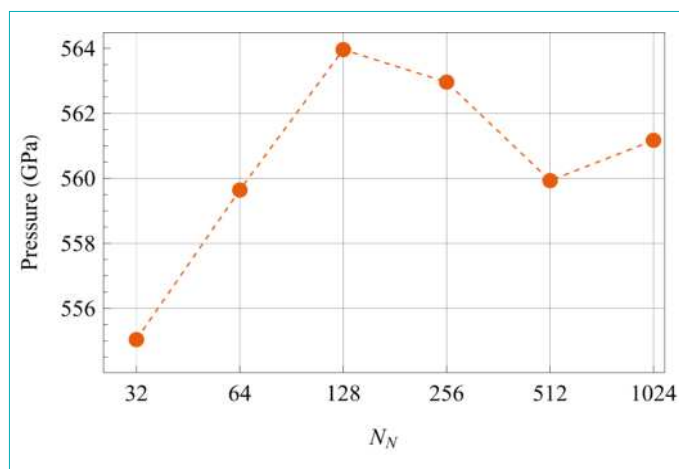


Figure 3. Average Hydrogen pressure as a function of system size. Each point represents a time average over a Langevin molecular-dynamics trajectory. The pressure converges with increasing system size, indicating that finite-size effects are small for systems of a few hundred atoms. Based on ref. [11].

quantities in the opposite ensemble. This demonstrates that, for the system sizes considered here, the two ensembles are effectively equivalent.

Figure 3 shows how the average pressure depends on system size. For small systems, noticeable finite-size effects are present, with the pressure increasing as more atoms are included. From about atoms onward, the pressure stabilizes within statistical uncertainty and remains nearly constant up to the largest systems studied. This indicates that finite-size and stochastic sampling effects are well controlled in this regime, and that the pressure is already representative of the thermodynamic limit.

The convergence of a transport property—the electrical conductivity (See Footnote 2)—is examined in Figure 4. At the lower density ($\rho=1 \text{ g cm}^{-3}$), finite-size effects are most pronounced for the smallest system, particularly at low frequencies. As the system size increases, the conductivity curves rapidly converge, becoming nearly indistinguishable for $N_H \geq 128$. The excellent agreement between the stochastic results and independent deterministic calculations performed on the same atomic configurations provides a direct validation of the stochastic approach. Note that, for the finite systems considered here, the deterministic approach does not yield a finite dc conductivity, whereas the stochastic formulation remains well behaved.

At the higher density ($\rho=16 \text{ g cm}^{-3}$), convergence is even faster. Conductivity curves for moderate system sizes already

overlap over the full frequency range, reflecting the more metallic character of the dense system.

Overall, these results show that equilibrium properties such as pressure converge relatively quickly with system size, while

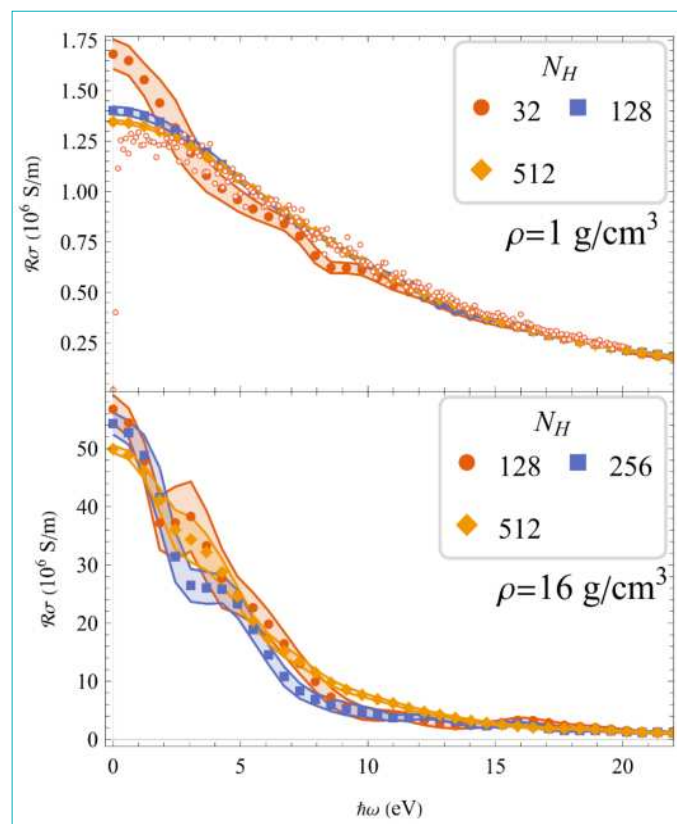


Figure 4. System-size frequency-dependent electrical conductivity of Hydrogen at the dependence of $T=30,000 \text{ K}$. The top (bottom) panel shows results at mass densities of ($\rho=1 \text{ g cm}^{-3}$) Each curve is averaged over multiple atomic configurations sampled along the molecular-dynamics trajectory. Statistical uncertainty is portrayed as a stained region. Results converge with increasing system size and at $\rho=1 \text{ g cm}^{-3}$ (for $\omega>0$) agree well with independent deterministic calculations shown as circles. Based on Ref. [11].

transport properties are more sensitive to finite-size effects, especially at low density and low frequency. Nevertheless, for system sizes of order a few hundred atoms, stochastic calculations yield reliable and well-converged results under the conditions studied here.

5. Summary and discussion

We began this work with a simple problem drawn from environmental monitoring: identifying correlations between

pollutants in a long and rapidly generated data stream. In that setting, storing and processing every measurement is impractical, yet the physically meaningful quantity—the correlation—can be recovered exactly by stochastic compression. By randomly projecting the data as it is generated and averaging over the resulting estimates, one can extract correlations on the fly without ever assembling the full dataset. This example illustrates a general principle: by accepting controlled randomness at the level of individual samples, it is possible to recover exact physical information on average while dramatically reducing computational and storage demands.

The same principle lies at the heart of the stochastic approach to electronic structure used here. Rather than explicitly computing and adding up contributions from an enormous number of electronic states, physical quantities are obtained by averaging over randomly constructed samples. Individual samples appear noisy, but their average converges steadily to the correct result.

Using stochastic density functional theory combined with Langevin molecular dynamics, we showed that this approach yields reliable equilibrium properties for warm dense hydrogen as a concrete case study. Although the forces and trajectories are noisy, the dynamics sample thermal equilibrium correctly. As a result, quantities such as temperature, pressure, and the equation of state are stable and reproducible, and different electronic ensembles give the same results within statistical uncertainty. Here, stochastic noise does not undermine accuracy; it is part of the sampling process.

Our analysis also highlights the role of system size. Equilibrium properties, such as the pressure, converge relatively quickly as the number of atoms increases. For systems containing a few hundred atoms, finite-size effects are already small. Transport properties, such as the electrical conductivity, are more sensitive and require larger systems, especially at low density. Even so, the stochastic approach achieves reliable results for system sizes that are far beyond the reach of conventional deterministic calculations.

At this point it is natural to ask how this approach differs from quantum Monte Carlo methods. While both use randomness, they do so in very different ways. In quantum Monte Carlo, random sampling is used to represent the full quantum state of the system, which can be extremely challenging and often leads to severe practical difficulties. In the present approach, randomness is used only as a computational tool to estimate physical quantities within an existing electronic-structure framework. The noise therefore reflects how the calculation is carried out, not a fundamental uncertainty in the quantum description itself. This distinction allows the

stochastic methods discussed here to scale efficiently to very large systems.

A key advantage of the stochastic framework is its flexibility. The same basic strategy applies to many different physical quantities, and accuracy can be improved simply by averaging over more samples. This makes it easy to balance precision against computational cost.

More broadly, the parallel between environmental data analysis and quantum electronic-structure calculations points to a shared computational philosophy. In both cases, the challenge is not too little information, but too much. Stochastic estimators provide a way to extract the essential physical content without being overwhelmed by microscopic detail. In recent years a plethora stochastic approaches have been developed to describe electronic structure of large systems [13-20].

In summary, stochastic estimators offer a simple and scalable bridge between microscopic models and macroscopic behavior. By treating randomness as a computational resource rather than a nuisance, they enable the study of correlations, thermodynamics, and transport in systems of unprecedented size and complexity.

Footnotes

1. Unless stated otherwise, all calculations presented below were performed for hydrogen at a temperature of $T=30,000$ K and a mass density of ($\rho=1$ g cm⁻³). The system is modeled as bulk hydrogen using a periodic cubic simulation cell, representing an infinite crystal. Brillouin-zone sampling is performed using a single Baldereschi k -point. The calculations follow the stochastic density functional theory framework described in [11].
2. Calculation of the electrical conductivity, within the Kubo-Greenwood theory, is also expedited considerably by using random vectors χ .

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CMC evaluation: ensuring quality in the pharma industry

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Introduction

My role at the Ministry of Health is called “CMC (Chemistry, Manufacturing, and Controls) dossier assessor.” During my degree studies, I studied medicinal organic chemistry, surfactant agents, electrochemistry, and chemical synthesis. In my professional career, I first worked in a R&D team at a start-up, then as a chief chemist in a large-scale industrial production company, and after a few years as head of the analytical team in the quality control (QC) department of a pharmaceutical company. As a professional possessing extensive accumulated and diverse knowledge in chemistry gained during both my academic studies and in various industrial capacities, I use this knowledge to analyze the information submitted regarding the quality of medicinal products.

In the modern pharmaceutical world, continuous product innovation requires strong regulation. The work of a “CMC dossier assessor” ensures maximum quality for the drugs reaching the public. The world’s leading quality requirements and regulatory standards are set by the FDA and the European Medicines Agency (EMA). These two giants establish policies that consist of constantly evolving regulations, and they also serve as approval bodies for specific products. The role of drug assessor in any country requires a deep understanding of chemistry, pharmacology, and regulatory aspects, which

is no less critical than the drug’s development itself. In this article, I will try to provide a glimpse into the work of a drug dossier assessor, focusing on the investigation of quality details of a medicinal product, detailing the necessary actions and important aspects in ensuring maximum quality, which ultimately affects every individual.

The submission of a medicinal product by a pharmaceutical company or its authorized marketer to a regulatory authority includes the submission of a “drug dossier,” which is essentially a comprehensive book containing all the information about the drug: its development, manufacturing, quality control, clinical trial results, drug stability and more. The structure of a regulatory dossier is fixed and uniform, according to MAH (Marketing Authorization Holder) requirements.

Quality dossier (CMC) assessment

The main aspects examined as part of a quality dossier investigation are as follows:

1. **Product Development:** This information details the reasons for selecting the product components, desired or limiting properties and trials conducted until the desired finished product is obtained.

Orit Ben Zazon (Gans) is a CMC dossier assessor in the Israel Ministry of Health. She completed a BSc in Medicinal Chemistry at Bar-Ilan University and had summer experience in Prof. Abraham Nudelman’s lab. She obtained an MSc in Applied Chemistry at the Hebrew University in Prof. Nissim Garti’s surfactants lab. She also studied electrochemistry at Ariel University. In industry, she worked in R&D at Sol-Gel Technologies, as chief chemist at Albaad wet wipes company and as QC team leader at CTS pharmaceutical company.



2. **Full information on Active Pharmaceutical Ingredients (APIs):** This includes complete synthesis of the APIs, Certificates of Analysis (CoAs) proving their purity, concentration, and absence of contaminants, information on suppliers and their compliance with Good Manufacturing Practice (GMP) standards, and an assessment of raw material stability under various storage conditions. These details about the active ingredients are often sent directly from the raw material manufacturers to the regulatory authority for review and are not visible to the finished product manufacturer.
3. **Manufacturing processes:** A detailed review of all production stages, from weighing and mixing to final packaging. The assessor ensures that the process is controlled, reproducible, operates under strict GMP conditions, especially at critical stages, and includes process validation, meaning verification that all important manufacturing steps have been properly validated, with results proving that the process consistently achieves the desired product.
4. **Quality control (QC):** This section consists of:
 - a. **Analytical methods:** Includes review and verification of the analytical methods used for drug quality control (e.g., HPLC, GC, spectroscopy). The assessor ensures that these methods have been validated, are specific, accurate, repeatable and have appropriate detection and quantification limits.
 - b. **Release specifications:** Verification of the specifications defining the quality of the final drug product before its release to the market, ensuring it meets all required parameters (such as appearance, pH, active ingredient concentration, dissolution, microbial purity).
 - c. **QC test results from multiple batches** to ensure consistency.
 - d. **Verification of reference materials** used for calibration and concentration determination, ensuring they have appropriate purity and quality.
 - e. **Degradation products and related impurities:** Identification and quantification of raw material residues, intermediates and degradation products formed during synthesis and under various storage conditions, ensuring they do not exceed permitted limits.
5. **Stability data according to stability protocols:** This includes storage conditions (temperature, humidity, light), test duration, and test methods. These data support the determination of shelf life, in-use shelf life and recommended storage conditions.
6. **Packaging materials and labeling quality:** Verification that packaging materials (bottles, blisters, caps, etc.)

do not react with the drug and do not compromise its stability.

This evaluation is designed to maximize patient safety by ensuring that the drug is safe for use and will not cause unexpected or severe side effects due to manufacturing defects or raw material issues. It also aims to ensure treatment efficacy, meaning that the drug delivers on its therapeutic promises and provides the desired effect according to its established guidelines. Furthermore, thorough examination of raw material sources and manufacturing processes will help prevent counterfeiting and contamination, thereby stopping the entry of counterfeit or contaminated materials into the supply chain.

The importance of chemistry expertise for the assessor's role

The core work of a CMC dossier assessor's relies on a deep understanding of chemistry. Knowledge of chemistry is not just an advantage, but a necessary condition for performing thorough and responsible work:

- **Understanding the structure and properties of materials:** Drugs are complex chemical molecules. An assessor with a background in organic chemistry understands the molecular structure of the API, its physicochemical properties (solubility, melting point, crystallinity), and the impact of these properties on drug stability, absorption in the body and efficacy. They can identify potential defects resulting from incorrect synthesis or the presence of impurities.
- **Analyzing manufacturing processes at a molecular level:** Drug manufacturing processes are inherently chemical processes. Chemical expertise allows the assessor to understand the rationale behind each step in the synthesis process, identify potential intermediates, assess the risk of unwanted byproduct formation, and audit the reaction conditions (temperature, pH, solvents) that affect the quality of the final product.
- **Evaluating analytical methods:** Quality control tests rely on chemical and analytical principles. A chemist assessor can critically assess the testing methods proposed in the dossier – whether they are specific enough, accurate enough, and sensitive enough to detect all potential **impurities** in the final product. They will understand the principles behind chromatography (HPLC, GC), spectroscopy (IR, UV, NMR), titrations, etc., and can ensure that method validation has been performed correctly.

- **Understanding drug stability and degradation chemistry:** Drugs are not infinitely stable. Chemistry expertise allows the assessor to understand possible chemical degradation mechanisms (hydrolysis, oxidation, photolysis, decarboxylation, etc.), identify expected degradants, and assess their impact on drug safety and efficacy. This knowledge is crucial for determining the correct shelf life and optimal storage conditions.
- **Compliance with regulatory requirements:** Many authorities require assessors to have deep chemical understanding to ensure drug quality. Chemical knowledge enables the assessor to “speak the same language” as the R&D, manufacturing, and QC teams of pharmaceutical companies, and to understand the scientific data they present.
- **Biomedical Engineering/Chemical Engineering:** Programs combining engineering knowledge with an understanding of manufacturing processes.

In addition to formal education, knowledge and experience in other important areas are required:

1. **Pharmaceutical Regulation:** Includes a deep familiarity with international pharmacopoeias and leading procedures of bodies such as the FDA, EMA, International Council for Harmonisation (ICH) and WHO. Also required is comprehensive knowledge of the requirements of the Israeli Ministry of Health, managed by the Pharmaceutical Division and the Institute for Standardization and Control of Medical Materials.
2. **Understanding of good manufacturing practices:** Deep knowledge of GMP requirements, which are strict standards for the manufacturing, packaging, storage, and quality control of drugs. The assessor must receive information and assess whether the manufacturer’s production processes comply with these standards.
3. **Advanced analytical chemistry:** Proficiency in analytical methods: theoretical and practical understanding of methods such as HPLC, GC, spectroscopy (UV-Vis, IR, Mass Spec, NMR), titrations, dissolution testing, and more. Ability to analyze test results and evaluate method validation.
4. **Drug stability and understanding degradation mechanisms:** Includes the ability to identify and analyze the chemical degradation mechanisms of active ingredients and the finished product under various environmental conditions.
5. **Quality assurance:** Familiarity with Quality Management Systems in the pharmaceutical industry, audit procedures, handling deviations, and controlled changes.

Without chemical expertise, a drug dossier assessor would be limited in their ability to review documentation without truly understanding the scientific complexity behind every number and process. They would not be able to ask incisive questions, identify hidden defects, or ensure that the drug is truly safe and effective. Therefore, chemistry is the scientific cornerstone upon which all the work of a drug dossier assessor rests, and it enables them to ensure the maximum quality of medicinal products reaching the public.

Qualification of a CMC dossier assessor

The knowledge of a CMC dossier assessor, with an emphasis on the quality aspects, is multidisciplinary and requires a variety of scientific fields, along with regulatory understanding and familiarity with pharmaceutical industry procedures. In Israel, the Ministry of Health is the MAH body.

Assessors are usually selected based on academic scientific background in one or more of the following areas:

- **Chemistry/Biochemistry:** This is the most critical scientific foundation. A deep understanding of analytical, organic, physical, and pharmaceutical chemistry is essential.
- **Pharmacy:** Pharmacy graduates acquire broad knowledge in pharmacology, industrial pharmacy, medicinal chemistry, and pharmacokinetics, all of which are relevant.
- **Biology/Biotechnology/Life Sciences:** These fields are relevant for evaluating biological products, vaccines and biotechnology-based drugs.

This means that a CMC dossier assessor in the quality field is a scientific expert with a background in chemistry who has completed specific training and specialization in pharmaceutical regulation and quality assurance. This is a job that requires precision, great responsibility, and an integrative understanding of complex processes to ensure the quality and safety of drugs reaching the public.

For pharmaceutical companies, the person submitting the drug dossier requires similar skills to those of a dossier assessor. Currently, in Israel, only a responsible pharmacist has the right to submit a drug dossier. Therefore, chemists

prepare dossiers but do not sign them and are thus not always involved in the process.

The importance of CMC dossier assessor

I will provide examples to show that even in the modern era, with advanced regulation, we still witness cases of poor-quality drugs, especially in unregulated markets or because of counterfeiting:

- **Drugs with no active ingredient/incorrect dosage:** Many counterfeit drugs contain little or no active ingredient at all, and sometimes contain harmful, toxic, or unknown substances that are not detailed on the product's label. For example, cases of cough syrup or children's vitamins, contaminated with diethylene glycol (DEG) or ethylene glycol (EG), can even lead to death. Another example is diabetic additives which contain metformin in various concentrations which are not mentioned in the product's insert. In Israel, the Pharmaceutical Crime Department buys and checks such drugs in order to remove counterfeit drugs from the market.
- **Contamination during manufacturing:** Failures in GMP conditions or manufacturing processes can lead to drug contamination with bacteria, heavy metals, or other toxic substances. For example, the case of the blood pressure drug 'Valsartan' where nitrosamine contaminants were found because of changes in the manufacturing process of raw materials, leading to a widespread global recall.
- **Substandard drugs:** These are drugs that do not meet the quality specifications or manufacturing standards set. They may contain an incorrect dosage of active ingredients (too little or too much), active ingredients of poor quality, or inactive ingredients that are unsuitable.
- **Falsified/counterfeit drugs:** In countries with weak regulation, the market is often flooded with counterfeit drugs. These drugs can contain no active ingredient, too little active ingredient, wrong active ingredients, or toxic substances. They may be sold in packaging that appears authentic, making identification difficult.
- **Danger to public health:** The consequences of substandard or falsified drugs can be catastrophic. They can lead to treatment failure, worsening of diseases, antibiotic resistance (in the case of low dosage), severe side effects, and even death.
- **Loss of trust in the healthcare system:** When the public loses trust in drugs and the healthcare system, they may avoid seeking medical treatment or risk unproven therapies.
- **Global challenges:** Today, drug supply chains are global. Drugs manufactured in poorly regulated countries can penetrate regulated markets through parallel imports or the black market, thereby endangering the health of populations in those countries.

These cases highlight the immense importance of thorough drug dossier evaluation, the scientific expertise of the assessors, and the need for continuous regulatory oversight, both before drug marketing and throughout its lifecycle. The consequences of poor quality in the pharmaceutical field can be life-threatening. This applies to drugs for humans sold in pharmacies as well as veterinary drugs for animals. As is known, some animals are later consumed as meat, and some live in homes as pets, so regulatory supervision of veterinary drugs is important to maintain human health as well.

Consequences of lack of strict regulatory requirements

While many countries require strict approval and control processes, there are also countries where regulatory requirements are weaker, or their enforcement is lacking. The main reason for these differences is, of course, economic. In these countries, drug quality can be significantly lower, with serious consequences for public health:

Sources of drugs in Israel

The drug market in Israel today combines significant local production with extensive imports. These are the places from which Israel acquires medicinal products:

1. **Local production:** Israeli pharmaceutical companies such as Dexcel Pharma, Rafa Laboratories, CTS, Perrigo Israel (formerly Agis), Rekah, Unipharm, Kamada, Madatech, and others, as well as Teva Pharmaceutical Industries, which manufactures drugs both in Israel and abroad. In addition, there are companies which produce veterinary drugs and vaccines, such as Fibro and BioVac.
 - **Generic drugs:** A significant portion of local production focuses on generic drugs, which are lower-priced alternatives to patented original drugs. These drugs must meet the same quality and safety standards as original drugs; their manufacturers are required to submit a dossier in which they must demonstrate quality and bio/therapeutic equivalence.

- **Original/Innovative drugs:** Only on rare occasions Israeli companies also engage in the development and production of innovative original drugs (such as Teva's Copaxone).
2. **Import of finished products:**
 - **Original and innovative drugs:** A large part of the original and innovative drugs included in the healthcare basket comes from leading international manufacturers located in countries with strict regulatory frameworks, especially Western Europe (such as Germany, Switzerland, UK) and the USA.
 - **Generic drugs** that are not produced in Israel or for some other reason need to be imported.
 3. **Import of API and pharmaceutical components:** There are a few companies in Israel that produce APIs, but a significant portion of the APIs and pharmaceutical components used in drug production – both in Israel and in Western countries – originate from China and India. The dependence on these sources exposes the global supply chain to risks in case of disruptions (such as the COVID-19 pandemic which highlighted this problem) but also requires strict oversight of the quality of APIs coming from these countries, even if they are not the manufacturers of the finished drug. Therefore, CMC dossier assessors carefully examine the API sources, claims, and documentation.
 4. **Special path:** It is possible to import unlicensed medical products to Israel, as well as to use registered drug in a manner inconsistent with their approved labeling. These are drugs for special cases, such as when there is no registered alternative in Israel, or in specific and urgent medical situations. These drugs are pursuant to the Ministry of Health guidelines number 29 (2007). They do not go through the long and secure dossier submission and evaluation process.

Following the digitalized world and the ability to order on websites, the Israeli Ministry of Health and international health organizations unequivocally emphasize: Do not purchase prescription drugs from the internet without an Israeli doctor's prescription, and only from a licensed pharmacy in Israel or abroad that is recognized by the Ministry of Health. Even for over-the-counter drugs and dietary supplements, it is recommended to purchase them

only from licensed pharmacies (physical or online) in Israel, which are closely supervised and provide pharmaceutical guidance. The dangers inherent in the "freedom" of online orders are real, can be fatal and clearly outweigh any perceived advantage of convenience or price.

Conclusion

Strict regulation is a necessary price for maintaining public health. The challenge is to find a delicate balance between ensuring safety and efficacy while shortening development times, reducing costs, and encouraging innovation. Regulatory authorities are aware of these drawbacks and are working to find ways to streamline processes, but this is a complex and ongoing task. One of the current activities is the efforts to establish mutual recognition with strict authorities such as the European Union, as has already been done regarding GMP procedures in Israel. Recognition will allow faster access to new drugs under optimal supervision, while maintaining a high level of quality.

The importance of this step lies in shortening times and, of course, this has significant economic implications. The danger inherent in incomplete inspection is that although the quality may be high, in practice, companies might classify batches for Israel that are not of the highest standards, or borderline batches that are not marketed in the West (as pharmaceutical companies do for production for third-world countries).

Conflict of interest and disclaimer

Conflict of Interest: The author declares no competing financial interests.

Disclaimer: The opinions and conclusions expressed in this manuscript are solely those of the author and do not necessarily reflect the official policy or position of the Ministry of Health. This review was conducted independently for academic and informational purposes and should not be construed as an official endorsement by the Ministry.

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Interview with Ilan Marek – recipient of the 2024 Richard Willstätter Lectureship

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Q: Where were you born and where did your parents come from?

A: I was born in Haifa, Israel, in 1963. My father, Eli Marek, had emigrated from Tunisia to Paris in the early 1950s, where he met my mother, Danièle. A passionate Zionist, he was deeply committed to contributing to the building of the State of Israel. In the late 1950s, they made *Aliyah* and settled in one of the few existing houses in Caesarea. Life in Israel at the time was rather austere, and my mother found it difficult to adjust—understandably so, as she had come from Paris, where life in the 1960s was vastly different. After several challenging years, my parents decided to return to Paris. In 1964, at the age of one, I flew with them to Paris, where I would spend the next 32 years of my life. Many years later, when my father returned to Israel and saw what Caesarea had become, he would often say, half-jokingly but with a trace of regret, that he should have stayed there!

Q: What and who inspired you to study chemistry?

A: To be honest, I wasn't particularly interested in chemistry during high school. What truly captured my attention were all activities outside the classroom—and I was pretty good at that! The only topic that hooked me at the time was deep sea exploration. The complete unknown of this universe. When I received my final secondary school diploma (the *baccalauréat* in France), I faced the question of what to study next. I quickly realized that, in the French academic system, becoming a deep-sea explorer meant pursuing geology, which I found absolutely unappealing.

So I shifted my focus to the opposite end of the scale—from the depths of the ocean to the vastness of the universe. I became captivated by the mysteries of cosmos, largely inspired by the writings of Canadian astrophysicist Hubert Reeves. That curiosity led me to enroll at the University Pierre et Marie Curie in a scientific program that combined mathematics, physics, chemistry, and biology.

At first, none of the subjects truly ignited my passion—until I took a course in organic chemistry taught by Professor Jean F.

Arlene Wilson-Gordon was born in Glasgow, Scotland. She completed her BSc (Hons) at Glasgow University and her DPhil at Oxford University under the supervision of Peter Atkins. After a postdoc at the Hebrew University with Raphy Levine, she joined the faculty at the Department of Chemistry, Bar-Ilan University, where she rose to the rank of Professor and in 2015, Professor Emerita. Her research interests lie in the field of theoretical quantum and nonlinear optics. She is the editor of the *Israel Chemist and Engineer*, an online magazine for all who are interested in chemistry and chemical engineering.



Normant. That was the turning point. From that moment on, I fell in love with organic synthesis—and the journey began.

Q: Why did you choose your particular field of chemistry?

A: To me, organic synthesis is far more than a scientific discipline—it is a form of art, a kind of craftsmanship at the molecular scale. Much like architects design structures that shape the physical world, synthetic chemists design and build molecules that influence the chemical landscape. The parallels between these two fields run deep. Both the architect and the chemist are governed by fundamental laws—gravity for one, quantum mechanics for the other—but within those boundaries, they are free to create with imagination. Just like a beautiful monument reflects the vision and creativity of its architect, the design of a new molecule—and the strategic path chosen to construct it—reveals the ingenuity of the chemist. In both cases, the outcome can be uninspired and awkward, or it can be breathtaking and profound. Whether working with steel and stone or atoms and bonds, the final creation stands as a testament to the author's imagination.

Both fields demand fluency in abstract thinking and spatial reasoning. Architects sketch blueprints, build models, and analyze forces; chemists draft molecular frameworks, simulate reactivity, and model electron flow. The transition from an idea to a tangible product requires mastery of both theory and technique.

Just as buildings are designed to withstand environmental forces—wind, temperature shifts, vibrations—molecules are shaped to respond to their surroundings. A molecule's behavior is dictated not only by its structure but also by its interaction with light, heat, solvents, and other molecules. Though they may appear static on paper, molecules are in constant motion—rotating, vibrating, and colliding in three-dimensional space.

The analogy extends even further. Molecules, like buildings, vary endlessly in form and function. Nature has constructed a vast catalog of complex molecules—plants, microbes, and marine life are all master builders in their own right. Human chemists, too, have contributed millions of new molecular “structures” to this catalog. In describing these, we often borrow the language of architecture: molecules have skeletons, frameworks, and branches; they are modified, decorated, and functionalized.

But functional groups are more than structural decorations—they define the “personality” of a molecule. They confer reactivity, determine physical properties, and influence how a molecule behaves in complex systems.

In both chemistry and architecture, the work is a fusion of aesthetics, functionality, and imagination. We build to understand. We build to solve. And, sometimes, we build simply because we can—because creation, at its core, is a deeply human endeavor.

So, from an aspiring deep-sea explorer to a dreamer captivated by the cosmos, I ultimately became an organic chemist—working with invisible molecular entities that, though unseen, possess the power to spark imagination, shape discovery, and reveal an undeniable aesthetic beauty.

Q: What do you consider to be your greatest scientific achievement, so far?

A: I am not sure I am the most qualified person to answer that question—I prefer to leave such judgments to the community. What I can say with certainty is that my enthusiasm, my excitement for new discoveries remains intact. No matter how many years pass, the excitement of the latest discovery always surpasses that of the ones before.

Q: What problems would you like to tackle in the near and far future?

A: There are so many questions that I would love to solve, I hardly know where to begin. Most of them revolve around chirality, stereochemistry, and the art of molecular design.

- Could we develop new, general, and reliable strategies to control stereochemistry for any S_N1 reactions?
- Could we find ways to deracemize multiple stereocenters along an aliphatic chain into a single enantiomer—all in a one-pot process?
- Could we achieve diastereo- and enantioselective 1,2-bisalkylation of alkenes?
- Could we devise methods to cleave carbon–carbon bonds with complete stereocontrol?
- Could we selectively functionalize alkanes—whether at the terminus or at a specific internal position—with full stereochemical control?

These are just a few of the questions that keep me up at night. And as each one would take years of dedicated research and a team of talented collaborators to solve, I have enough to keep me busy for the next 30 years!

Q: Would you recommend a career in academia to young scientists?

A: Absolutely, this is among the most rewarding career one can pursue. It requires a touch of naivety and idealism, but above all, a strong drive and an insatiable curiosity. The rest tends to follow naturally.

Q: What are the main challenges facing Israeli science?

A: Stability, understanding and support!

Q: What do you consider to be your greatest contribution to Israeli society?

A: After spending many years developing and enjoying my own research, I decided a few years ago that it was time to create something that would be useful for Israeli society. As one of the most urgent challenges is to develop new catalytic processes that are sustainable and do not harm the environment, I devoted rather a large amount of my time to establish the **Resnick Sustainability Center for Catalysis** thanks to generous support from Stewart and Lynda Resnick. Since a large range of industries engage in catalysis as part of their production processes, it is imperative to develop effective solutions that promote clean technologies and a more sustainable world. This unique Center will advance the development and dissemination of innovative catalysis knowledge and technologies, thereby contributing to a more sustainable world.

The Resnick Sustainability Center for Catalysis will be established to discover and develop new catalysts and catalytic processes to deal with the enormous challenges the world currently faces. This will be achieved by combining and harnessing initially the Technion's outstanding resources in such disciplines as Chemistry, Biotechnology and Food Engineering, Biology, Chemical Engineering, Materials Sciences and Engineering, Architecture, Civil and Environmental Engineering, Mechanical Engineering, Aerospace Engineering and Electrical Engineering, all within a single facility.

The new Center aims to foster interdisciplinary relationships and to create a collaborative enterprise among scientists from a large range of disciplines. Working together, these scientists can conduct excellent, high impact research aimed at developing new synthetic methodologies and coherent theories, employing rational design. This will mark the end of an era characterized primarily by trial-and-error and establish new fields of study hallmarked by directed catalyst design for sustainable process development.

In addition to serving as a physical hub for state-of-the-art multidisciplinary research, the Resnick Sustainability Center for Catalysis will nurture a broad community of excellent

scientists and cultivate the next generation of leadership among catalysis researchers. It will act as both a national and international center of advanced catalysis-related activities, proactively encouraging the development of innovative and creative technologies that will lead to more sustainable practices around the world.

The Resnick Center will be the only one of its kind in Israel, based on an underlying faith in the value of interdisciplinary research for achieving scientific and technological breakthroughs. As such, the Center will operate according to an innovative model that encourages physical and intellectual interaction among researchers from diverse fields of expertise committed to fostering sustainability and responsible research practices.

This vision will be fulfilled through the introduction of innovative programs and initiatives. First and foremost, the Center will serve as an incubator for outstanding young faculty members whose fields of expertise are relevant to the advancement of new forms of catalysis. The incubator will nurture eight new faculty members at a time; they will conduct research at the Center for a six-year period, after which they will receive tenure at their home faculties within the Technion.

Another key element that defines the Center's *raison d'être* is the desire to connect between academia and industry. Indeed, the center will encourage companies – from start-ups to multinationals, local as well as international – to consult with it on the subject of sustainable catalysis. Moreover, it will nurture new start-ups and spinoffs, providing valuable help during their scale-up phases thanks to accelerated discovery in the Center's labs. In this way, the Resnick Center will play an active role in boosting the attractiveness of start-ups for prospective investors.

Q: If you had a magic wand, what would you change in academic life?

In the realm of academic work (chemistry), one of our most cherished and enduring strengths lies in the human relationships among researchers across Israel. This vibrant community, mutual support, collegiality, and a commitment to excellence, is a cornerstone of our scientific achievements. I am very proud of my colleagues and of their achievements! Preserving and nurturing these connections is essential.

However, to sustain and elevate our scientific endeavors, there is a pressing need for enhanced institutional support. Faculty members often find themselves juggling multiple (too many) responsibilities, within the confines of a 24-hour day! This

multifaceted workload can impede the depth and breadth of research activities.

Our international competitors frequently operate within frameworks that provide substantial technical and administrative assistance, enabling them to focus more intently on research innovation. In contrast, Israeli researchers, particularly at the mid-career stage, may encounter limitations in accessing resources necessary for advancing their work. While early-career researchers often benefit from initial generous funding and support, sustaining momentum into mid-career requires renewed investment in equipment, personnel, and infrastructure, that is not easy.

To maintain our competitive edge and continue contributing significantly to global scientific discourse, it is imperative to provide sustained support that addresses the unique needs of researchers at this pivotal stage. By doing so, we can ensure that the Israeli scientific community remains dynamic, and at the forefront of innovation.

Q: How do you enjoy your free time?

A: Traveling with my family and hopefully enjoying the quietness and beauty of a deserted Greek island.

Interview with David Avnir – recipient of the 2024 ICS Gold Medal

Arlene D. Wilson-Gordon

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Q: Where were you born and where did your parents come from?

A: I was born in 1947 in a Displaced Persons hospital at the Benedictine archabbey of St. Ottilien, Germany. In 1949 we made aliya to Israel. My mother is from Warsaw, and my father from a small village, Ratna, then in Poland and today in the Ukraine.

Q: What and who inspired you to study chemistry?

A: I was born a scientist, and already carried out “chemistry” experiments, at the age of 3.

Q: Why did you choose your particular field in chemistry?

A: I have been active in several fields of chemistry – see https://en.wikipedia.org/wiki/David_Avnir for details. Selection of these fields has always been motivated by searching for question marks that, by-and-large, were original or touched upon only marginally before.

Q: What do you consider to be your greatest scientific achievement, so far?

A: As mentioned above, I have been active in quite a wide range of fields, both experimental and theoretical, and “I love all my children equally.” Anyway, some of the main contributions in each of these fields have been the merging of organic chemistry with the chemistry of ceramics and glasses; the introduction of the concept that symmetry is not only a feature which either exists or not, but has continuous properties; the ability to incorporate organic molecules within metals; the ability to treat complex geometries of materials on the molecular level, by using fractal geometry;

the development of a wide range of methods to introduce chirality in materials; and more.

Q: What problems would you like to tackle in the near and far future?

A: I have recently entered the fields of astrochemistry and geochemistry, where I mainly investigate the possible relation between the existence of chiral materials and molecules (chirality: the existence of left-handed and right-handed versions of the same) in space, and the phenomenon of chirality of Life on Earth and possibly elsewhere. As for the far (or perhaps not so far) future, it is intriguing to explore what are the horizons and limitations of the use of artificial intelligence, for the whole of chemical research.

Q: Do you enjoy teaching and interacting with students?

A: Yes, and I quite often received high marks from students, which has been a valuable recognition for me.

Q: Would you recommend a career in academia to young scientists?

A: My approach has always been to tailor my advice to the specific personality and strengths of the person, be it academia, industry, teaching, science administration, business management, and so on.

Q: What are the main challenges facing Israeli science?

A: Raising adequate research funds; improving the level of science learning in high-schools; and recently, unfortunately, facing the increasing number of cases of boycotting Israeli scientists in various open and concealed ways.

Q: What do you consider to be your greatest contribution to Israeli society?

A: Putting Israeli chemistry on the global arena.

Q: If you had a magic wand, what would you change in academic life?

A: Major increase in the funding of basic science which does not ask “What is it good for?” but is motivated by curiosity alone.

Q: Do you have any advice for young people embarking on their career?

A: Most of all, to try to do the best in one’s activity; and to understand that failures are never a reason to give up.

Q: How do you enjoy your free time?

A: Who said I have free time?

Interview with David Cahen – recipient of the 2024 ICS Gold Medal

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Q: Where were you born and where did your parents come from?

A: I was born in a village in the “deep south” of the Netherlands; my ancestors can be traced to early 19th century Germany (early 17th century from Alsace; Cahen) and Portugal & Palestine (17th century; Rodriguez de Miranda & Elion).

Q: What and who inspired you to study chemistry?

A: Around the age of 8–9, I became hooked on science (I distinctly remember trying to keep cutting my piece of cheese to get to an “atom” of cheese and this was before I started classical Greek...). I was probably inspired by the one good science teacher I had for first-year chemistry (10th grade) in high school, Niels Wiedenhof.

Q: Why did you choose your particular field of chemistry?

A: It must have been during the first half of the third year of my undergraduate degree at the Hebrew University of Jerusalem, possibly as a counter-reaction to the heavy organic chem lab we all (even those in the Chemistry + Physics program) had to do (“courtesy” of Ernst David Bergmann) that I was not particularly fond of. To his great credit, the late Johanan Blum who was one of the lab teachers (the other was the late Zeev Aizenshtat) tolerated it. Johanan must have seen something in me that I did not, as otherwise I do not know how I got accepted to Northwestern (strong materials center) for a PhD that in the end was joint chemistry and materials science.

Q: What do you consider to be your greatest scientific achievement, so far?

A: 1. DOPING of semiconductors via their surfaces. We realized that in polycrystalline thin films of the type used in most macro-electronics, bulk electronic doping will be first via their surfaces, rather than by introducing dopants inside the grains. We proved this and showed the opportunities it provides (originally with Rommel Noufi; later also with Antoine Kahn).

2. Discovering SELF-HEALING of inorganic compounds, especially semiconductors (originally with Leor Kronik and others; later with Gary Hodes, Davide Ceratti, Dan Oron and others).

3. Discovering that PROTEINS can be quite good electronic conductors (with Mordechai Sheves and Israel Pecht).

Q: What problems would you like to tackle in the near and far future?

A: 1. Get to the bottom of the necessary conditions for self-healing, especially in materials for energy conversion and storage (out of curiosity and for our own sake, i.e., sustainability).

2. Find the mechanism that allows efficient electron transport through proteins, which still is a riddle.

Q: Do you enjoy teaching and interacting with students?

A: Yes

Q: Would you recommend a career in academia to young scientists?

A: Obviously, I cannot be objective here, as I chose this path AND I spent most of my career in the Weizmann Institute bubble. Also, former students and postdocs have made and are making great careers in academia and in industry. Today in academia one needs skills beyond the ones I had when I joined as, in hindsight, I had no idea of what was expected, beyond doing original research (without any guidance or mentorship). Apart from being creative and preferably also proficient in your areas of choice, you need self-confidence and an open mind to listen to and then analyze criticism, and to withstand the often petty jealousies in academia that put to shame the goal of research as I see it: successively better approximations to what we see at a given point in time as “truth.” Exact scientists, especially, must be able to forego a pet model that may even have brought them fame, if new experimental results and/or logical reasoning shows it to be wrong.

Q: What are the main challenges facing Israeli science?

A: 1. Research funding here, as everywhere else, is one of the easiest budgets to cut. We had a reasonably good defensive barrier between this and politics, but in the last decade(s) efforts to dismantle that shield have increased to the point that tomorrow it can be annihilated. At this point, it is still mainly the humanities and social sciences that are under attack, but I remember well the Latin proverb (Horatius) that “greeted” me whenever I entered my high school, “*Tum tua res agitur, paries cum proximus ardet* (You too are in danger, when your neighbour’s house is on fire).” At least, until now, most exact science colleagues understand this. While certainly not unique to Israel, here we also lack the checks and balances to dampen the effect.

2. As I mention in my previous answer (and noted separately by David Mermin and Steven Weinberg, among others, I assume), one thing you must be able to do as a scientist is to forego use of the model or theory or mechanism that you found or used, when a new experimental result or theoretical development shows it to be wrong. Thus, the continuing down-grading of the

concept of “fact,” seems to me especially problematic for the so-called “hard” sciences.

Q: What do you consider to be your greatest contribution to Israeli society?

A: Spreading the word about the need for sustainable resources, energy and materials, something that became clear and dear to me when I read “Limits to Growth” (Donnella Meadows, Jorgen Randers, and Dennis Meadows) and “the Waste Makers” (Vance Packard) during my PhD.

Q: If you had a magic wand, what would you change a) in academic life, b) in Israeli society?

A: In academia, as we are a small place, we still have a way to go in decreasing the often barely noticed role of academic genealogy in our evaluations (although, I doubt that being academic great grandchild of Linus Pauling ever affected me for better or worse; it was not at all local).

In Israel: we need a constitution, rather than the present make-believe system.

Q: Do you have any advice for young people embarking on their career?

A: Read Peter Medawar’s “Advice to the Young Scientist,” from which I can (more or less) quote that when you choose a problem to research, make sure that if you solve it, it will matter (in as far as you can judge at the time).

Q: How do you enjoy your free time?

A: Reading history (if I had gone to a liberal arts college, I would probably have taken it as my minor), travelling, walking and... trying to improve my *Haaretz*’s weekly 20 questions score.

For more insights, see

<https://communities.springernature.com/posts/the-sceptical-chymist-reactions-david-cahen>

The 88th Annual Meeting of the Israel Chemical Society: February 18–19, 2025, International Convention Center, Jerusalem, Israel

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Taly Lidor,
CEO of the ICS



Ehud Keinan,
President of the ICS.

Introduction

The Annual Meeting of the Israel Chemical Society (ICS) has a long history, dating back to its establishment in 1933, and is a well-known event in the scientific landscape of the State of Israel. These colorful gatherings of Israeli chemists usually take place in mid-February, during the inter-semester break at all Israeli universities.

Following ICS tradition, the chemistry departments of the six major research universities share responsibility for organizing these meetings in a six-year cycle, in the same order: the Hebrew University of Jerusalem, Technion, Tel Aviv University, Bar-Ilan University, Ben-Gurion University of the Negev, and the Weizmann Institute of Science. Following a decision of the ICS Executive Board, Ariel University joined this cycle in 2024 and organized the 87th ICS meeting on April 3, 2024. Thus, looking back over the past two decades of ICS history, Bar-Ilan University has taken responsibility for organizing the 70th Meeting (2005), the 76th Meeting (2011), the 82nd Meeting (2017), and the 88th Meeting (2025).

Another unique tradition the ICS has followed for more than 25 years is hosting high-profile delegations of distinguished scientists from top academic institutions worldwide to deliver plenary and keynote lectures. This tradition has created outstanding opportunities for many Israeli scientists, particularly graduate students, to interact with world-renowned chemists, thereby enhancing networking and scientific collaboration. Unfortunately, the large delegation of 10 scientists and 20 graduate students from the leading

universities in Taiwan could not participate due to the ongoing war in Israel.

Nevertheless, it provided an opportunity for a happy gathering of many students and scientists from around Israel, even in the absence of a foreign delegation. Over 700 participants enjoyed a diverse scientific program that included two plenary lectures. The five parallel session halls included 16 keynote lectures, 99 invited lectures, and 66 flash talks. The 304 posters were distributed between two poster sessions, and four were selected to receive the best poster prizes, announced at the closing ceremony.

The parallel sessions of the first day (Figures 1 and 2) included Organic and Organometallic Chemistry (organized by Samer Gnaim of the Weizmann Institute, & Alex Szpilman from Ariel University, Bio-organic & Bio-inorganic Chemistry (organized by Galia Maayan of The Technion), Physical Chemistry (organized by Assaf Ben Moshe of Bar-Ilan University, Energy & Electrochemistry (organized by Diana Golodnitsky of Tel Aviv University, & Hannah Noa-Barad from Bar-Ilan University), Medicinal Chemistry (organized by Eylon Yavin from the Hebrew University of Jerusalem), Inorganic Chemistry & Catalysis (organized by Idan Hod from Ben-Gurion University), and Chemical Education (organized by Tamar Traube of Bar-Ilan University & Dorit Taitelbaum from the Ministry of Education).

The parallel sessions of the second day included Polymer Chemistry (organized by Roy Shenhar of the Hebrew University of Jerusalem), Nanoscience & Advanced Materials



Figure 1. A collage of photos reflecting the general atmosphere throughout the 88th ICS meeting, including the lectures, posters, and commercial exhibition. Photos by Dror Sithakol.

(organized by Fernando Patolsky of Tel Aviv University & Taleb Mokari from Ben-Gurion University), Agricultural and Food Chemistry (organized by Elena Poverenov of the Volcani Institute), Spectroscopy & Analytical Chemistry (organized by Sharly Fleischer from Tel Aviv University), Theoretical Chemistry (organized by Amikam Levy from Bar-Ilan University), Innovative Industrial Chemistry (organized by Itsik Bar-Nahum from ADAMA), Supramolecular Chemistry (organized by Boris Rybtchinski from the Weizmann Institute), Soft Matter & Colloidal Chemistry & Biophysics (organized by Bat-El Pinchasik from Tel Aviv University).

In addition to the scientific program, the ICS held its traditional General Assembly on the afternoon of the first day, discussing the past year's activities, plans for the next year, and financial issues. Mr. Shimon Nizrad, the ICS accountant, provided an overview of the ICS's budget, legal status, and financial goals. The prize ceremony, which took place on the evening of the first day, was preceded by a reception and light dinner for all the participants.

The event attracted many sponsors, including the Weizmann Institute of Science, Tel Aviv University, Bar-Ilan University, Ben-Gurion University of the Negev, the Hebrew University of Jerusalem, Ariel University, the Open University, and the Technion. The experienced team of the ICS production department, led by Taly Lidor, took responsibility for the actual operation, including all technical aspects, administration, exhibition organization, promotion, etc.

The meeting included a commercial exhibition by 20 suppliers of lab equipment, scientific instrumentation, chemicals, materials, analytical chemistry services, publishing houses, and intellectual property management. Exhibitors included Arad-Ophir Information Specialists Ltd., Bargal Analytical Instruments Ltd., BioAnalytics Ltd., Bruker Scientific Israel Ltd., Meshulam Avni & Son Ltd., Labotal Scientific Equipment Ltd., LabSuit Projects Ltd., Mark Technologies Ltd., Mercury Ltd., Dr. Golik Scientific Solutions Ltd., Rhenium Ltd., and Tzamal D-Chem Laboratories Ltd.

This mix of excellent lectures, colorful poster sessions, exhibitions, and other activities created a vibrant atmosphere, with lively discussions, information exchange, and social gatherings, as reflected in the collage of photographs (Figures 1 and 2).

Opening Ceremony

Prof. Gerardo Byk, co-chairperson of the organizing committee, opened the meeting and greeted the guests and participants: "Good morning, everyone, it's a pleasure to welcome you all to the 88th ICS meeting. I'm excited to have

so many brilliant minds gathered here to share ideas, insights, and breakthroughs in the fascinating world of chemistry.

Before we begin, I would like to take a moment to address the tragic events of October 7th. The horrific attack on Israel that day resulted in devastating loss and suffering, and many lives were affected. Among those impacted are our fellow chemists, researchers, and members of the scientific community. Some have lost loved ones; others have had their lives and work disrupted in unimaginable ways. Our thoughts are with all of them, and we stand in solidarity with our colleagues and citizens who are enduring this hardship.

In times of crisis like this, it's important to remember the power of community and support. As chemists, we know the value of collaboration, and it's during difficult times like these that our bonds with one another are most crucial. The scientific community is global, and we must continue to support and uplift one another, especially those facing such unimaginable challenges.

Turning to today's meeting, we are reminded of the importance of the work we do. Chemistry is not just a science; it is a tool for progress, healing, and understanding. Whether it's developing solutions to global health issues or tackling environmental challenges, chemistry has the potential to make a meaningful difference in the world.

Gathering at the 88th ICS meeting is an opportunity for us to collaborate, share ideas, and continue advancing our collective mission to create positive change. To ensure balanced representation of institutions and genders, we established an ad hoc scientific committee composed of representatives from all relevant institutions and areas of expertise in chemistry. This committee was tasked with overseeing the meeting's organization. To facilitate the process, the committee appointed session chairs, who were responsible for curating the program. This included selecting speakers and reviewing and approving posters and flash talks. This structure ensured a fair and inclusive approach, fostering a collaborative and diverse scientific environment throughout the event.

This year, we are excited to welcome over 600 registered participants, with a program featuring around 220 talks, including more than 70 flash talks by students and post-doctoral researchers, and over 300 posters. Additionally, two roundtable discussions have been scheduled to address pressing topics in chemistry.

I eagerly anticipate the presentations and discussions that lie ahead, and I hope the 88th ICS meeting serves as a reminder

of the strength and resilience of our scientific community, both in times of peace and in times of challenge.

With that, my co-chair, Hagay Shpaisman, and I would like to open the meeting officially. Thank you for being here, and I look forward to the inspiring conversations and groundbreaking discoveries that await us today.”

Prof. Ehud Keinan, president of the ICS, added his greetings: “Good morning, everybody, and welcome to the 88th Meeting of the ICS. First, I would like to thank all the people who made it possible: chairpersons Gerardo Byk and Hagay Shpaisman, and their colleagues from Bar-Ilan University; the ICS CEO, Tali Lidor; and the members of the organizing committee and session organizers. Special thanks go to the sponsors, who made this event possible.

The past five years, including the COVID-19 lockdown followed by the longest war in Israel’s history, presented unusual challenges to the ICS, forcing change and postponement of our annual meetings, and serial cancellations of various programs. After losing the opportunity to host a large delegation of 30 scientists from China due to the COVID-19 pandemic, we looked forward to hosting a large delegation from Denmark, including 10 professors and 20 graduate students from the three top Danish universities. Unfortunately, the long war in the Middle East cancelled not only the arrival of the Danish delegation, but also two alternative attempts to bring in delegations from the chemical societies of Switzerland and Taiwan. I hope that we’ll be able to return to the normal schedule and continue this tradition of hosting large delegations from abroad.

The current political situation in Israel may not allow for inviting a delegation for the next meeting. Still, I am happy to announce that the 89th annual meeting will be held in February 2026 under the responsibility of Tel Aviv University, with Roey Amir and Yuval Ebenstein co-chairing the event.

Since this is my second year as IUPAC President, I take this opportunity to remind you of several significant IUPAC awards. The newly established IUPAC-Soong Prize for Sustainable Chemistry is a high-profile award that includes a medal, a \$30,000 monetary award, and travel expenses to attend the prize ceremony. We plan to award it annually, and the inaugural ceremony will take place in July 2025. We still accept nominations for the IUPAC Top Ten Emerging Technologies in Chemistry 2025, including self-nominations. The IUPAC Distinguished Women in Chemistry or Chemical Engineering biennial award recognizes women scientists, educators, and engineers worldwide.

As Editor-in-Chief of the Israel Journal of Chemistry, I encourage all ICS members to consider highlighting a specific chemistry topic by guest editing a special issue of the journal. I’ll be happy discussing your proposals and the optimal timeline.

I’m happy to see the many enthusiastic young people eager to resume the Annual Meeting and meet friends and colleagues from around the country. Thanks again for participating in the 88th ICS Meeting; I wish you an enjoyable, highly fruitful experience!”

Plenary lectures

Efrat Lifshitz of the Technion, the ICS Prize of Excellence winner, lectured on “Spins in the Wonderland of Semiconductor Nanostructures.” She explained that unpaired spins in solid or soft materials serve as spectators of local chemical environments, mutual dipole interactions, and structural anisotropy. At the same time, the unpaired spins dictate the fundamental optical, magnetic, and quantum properties of hosting materials. She provided selective examples that demonstrate the influence of individual or collective spins (magnetism) on the electronic and optical properties of low-dimensional materials, intentional magnetic or self-doping in II-VI colloidal quantum dots, long-range magnetic order in metal phosphor tri-chalcogenide compounds, and intrinsic magnetism in perovskite materials. Overall, the observations underscore the fundamental role of spins in governing the optical and magnetic properties of low-dimensional semiconductors, with significant implications for the development of modern spin-electronics and spin-optical devices.

Roi Baer of the Hebrew University of Jerusalem, the ICS Prize of Excellence winner, lectured on “Stochastic Approaches to Computational Electronic Structure and Dynamics in Materials.” He explained that computational electronic structure theory plays a pivotal role in understanding and predicting processes and properties of materials, such as catalytic activity, electrical conductivity, light-harvesting efficiency, thermal transport, and magnetic behavior. It applies equally to materials in our everyday lives as to probing matter under extreme conditions, as in planetary cores and inertial confinement fusion. These theories combine quantum mechanics and Fermi particle statistics and must address extensive systems involving thousands of electrons. Challenges arise from approximations, which often introduce errors, since accurate calculations for large, complex systems are prohibitively expensive.

Furthermore, describing excited states, multiparticle excitations, and mesoscopic systems requires intricate

quantum many-body approaches. Baer presented stochastic approaches as a powerful and innovative framework for addressing these challenges. Specific applications included ab initio molecular dynamics for warm dense matter, Green's function theory for charge-carrier energies in semiconducting nanocrystals, excited-state dynamics, and open-system dynamics, including dissipation and decoherence processes.

Keynote lectures

Moshe Portnoy of the School of Tel Aviv University, lectured on "Expanding the Span of Site Selectivity in Modifications of Amphiphilic Diols: from New Nucleophilic Catalysts to Amine Base Promoters."

Gary Gellerman of Ariel University spoke about "Antibody-driven sonodynamic therapy as a novel approach to target cancer."

Daniella Goldfarb of the Weizmann Institute of Science spoke about "Interaction of Magnetic Field with Diamagnetic Liquids."

Doron Aurbach of Chemistry, Bar-Ilan University lectured on "Electrochemical and chemical cycles for decoupled water electrolysis."

Mark Gandelman of the Technion spoke about "Novel Strategies for (Asymmetric Catalytic) Synthesis of Halo-organic Compounds."

Moran Shalev-Benami of the Weizmann Institute of Science, winner of the 2024 ICS Prize for Outstanding Young Scientist, lectured on "Targeting A β oligomers for early theranostics of Alzheimer's disease."

Ira Weinstock of Ben-Gurion University of the Negev lectured on "Solution-State Chemistry of Polyoxometalate-Complexed Oxides."

Maya Bar Sadan of Ben Gurion University lectured on "Innovative Phosphides for Enhanced Hydrogen Evolution and Alcohol Oxidation Reactions."

Elizabeth Amir of the Shenkar college spoke about "Chemical grafting of biopolymers as a tool for fabrication of functional materials."

Ron Naaman of the Weizmann Institute spoke about "Chirality and the electron spin- A miraculous match."

Joshua Baraban of Ben-Gurion University, winner of the 2024 ICS Prize for Outstanding Young Scientist, spoke about "New Spectroscopic Strategies for Reactive Molecules."

Ronnie Kosloff of the Hebrew University spoke about "Quantum open systems dynamics: two approaches to thermodynamically consistent driven master equations".

Yitzhak Mastai of Bar-Ilan University lectured on "Chiral nanostructured materials."

Gil Markovich of Tel Aviv University spoke about "High enantioselectivity in adsorption of chiral molecules on the surface of chiral terbium phosphate nanocrystals."

Kinneret Keren of the Technion lectured on "Topological Defects and their Role in Hydra Morphogenesis."

Oded Shoseyov of The Faculty of Agriculture Food and Environment, The Hebrew University of Jerusalem spoke about "The Plant Age; Materials for the Future; Nature's Gift."

The ICS Awards Ceremony

Following ICS tradition, all prize winners (Figures 3 and 4) received their awards at the special ceremony held on the evening of Tuesday, February 18, 2025, after the reception.

The 2024 ICS Prize for an Excellent Graduate Student was awarded to seven excellent students in alphabetical order by the ICS president and a representative of the relevant university:

Anastasia Behar was born in 1989, raised in Kherson, Ukraine, and obtained her BSc in Analytical Chemistry (2011) from Odesa I. I. Mechnikov National University. She made Aliya on her own (2017), started her MSc at the Technion with Prof. Galia Maayan's group (2018), and continued to a direct-track PhD (2019). Her research focuses on peptoid-based chelators for selective copper binding in therapeutic applications. She has developed the first peptoid-based ligand that competes with the copper-amyloid complex for copper and prevents its mediated reactive oxygen species production associated with Alzheimer's disease etiology (*Angewandte Chemie*, 2021). She received several awards for excellence in teaching and faculty academic excellence and was shortlisted among the top 15 female PhD students at the Technion (2023). She will shortly begin her ANR-funded postdoctoral research at École Normale Supérieure and Sorbonne University (Paris, France), where she will work on the targeted delivery of catalytic metal-based SOD mimics for anti-inflammatory therapies.



Figure 2. A collage of photos reflecting the general atmosphere throughout the 88th ICS meeting, including the lectures, posters, and commercial exhibition. Photos by Dror Sithakol.

Roey Ben David was born in 1990 in Holon and raised in Rishon LeZion. He received his BSc in Materials Engineering and Chemistry from the Technion (Summa Cum Laude, 2013) via the Atuda program. During his undergraduate studies, Roey worked as a process engineer in the micro-electromechanical systems (MEMS) department at RAFAEL. After graduating, he was a researcher at the Israel Atomic Energy Commission (2013-2019). He completed his MSc in Materials Science and Engineering and MSc in hydrogen interaction with metals and hydrogen storage materials. For his PhD, he joined Dr. Baran Eren (2019) at the Weizmann Institute, exploring the gas-solid interface of model catalytic systems under ambient temperatures and pressure using in-situ surface-sensitive spectroscopic techniques. His work has elucidated the atomistic mechanisms of catalytic methanol decomposition, carbon dioxide activation, and hydrogenation. Roey has received the Schulich Excellence Prize in Chemistry, the Rosen Excellence Prize in Materials Engineering, and the Israel Vacuum Society (IVS) Excellence Award for Outstanding PhD Student (2023), the Moshe Meir Horwitz Memorial Fellowship, the Yoel Meches Fellowship, and the Ministry of Energy PhD Fellowship.

Asmita Dutta joined the Department of Chemical Sciences at Ariel University in 2020. Her PhD research focused on new synthetic methods for advanced carbon-based composite materials, titled “Structural Modification of Carbon-based Nanomaterials,” under Dr. Arie Borenstein. She presented her findings at various scientific meetings despite the challenges posed by the COVID-19 pandemic, including the Israel Vacuum Society (IVS), Israel Electrochemistry (ISLE), NATI, and international conferences in Poland and the Czech Republic. Asmita published eight papers, and two others are now under review. She earned the 3rd-place PhD Excellence Award for the academic year 2022-2023 at Ariel University.

Nadim Eghbarieh was born in Musmus village (1995), obtained his BSc in Chemistry and Biology at The Hebrew University (2019), and continued to PhD on a direct track under Prof. Ahmad Masarwa. His research focuses on new synthetic methodologies and reactive species, including catalysis, photochemistry, polymer chemistry, and drug discovery. He studied the reactivity and applications of polyborylated compounds and organoboron-based motifs that contain multiple boryl groups. He studied the elusive α -bimetallic-carbon-based radical and applied it to many previously unknown transformations. Nadim published 11 articles in leading journals, such as Nature Communications, JACS, and Angew. Chem. He received the Neubauer Fellowship for outstanding PhD students, the ICS Prize for the best poster (2020), and the Kathleen Casali Fellowship in Applied Chemistry (2020 and 2021).

Omri Shelef was born in Tel Aviv in 1994. He obtained his BSc in Chemistry and Biology (2019) from Tel Aviv University and continued to a direct-track PhD under Prof. Doron Shabat. His research focuses on developing chemiluminescent (CL) diagnostic tools to improve disease diagnosis through highly sensitive, cost-effective, and user-friendly solutions. Leveraging fundamental synthetic organic chemistry, Omri has created innovative CL probes for detecting viral infections, bacterial pathogens, and cancer, including a high-throughput antiviral drug screening platform and a robust system for microbial identification. His contributions have challenged long-standing assumptions in his field, earning him recognition through the Adams Fellowship and the Gertner Institute for Medical Nanosystems Excellence Student Award. Omri is also passionate about education and science communication, having been recognized as one of Tel Aviv University’s Top 100 Teachers/Lecturers and authored reviews on self-immolative polymers and CL probes.

Rifael Snitkoff-Sol received his BSc in Chemical Engineering (cum laude) at Shenkar College, MSc (summa cum laude), and PhD in Chemistry at Bar-Ilan University under Prof. Lior Elbaz. His research focuses on novel methodologies for analyzing platinum-group metal-free electrocatalysts. He developed an in-situ technique for analyzing catalysts during fuel-cell measurements and methods for analyzing electrocatalytic reactions using Fourier-transformed ac voltammetry and microkinetic modeling. He has published six first-authored papers, two in Nature Catalysis, and co-authored six additional articles. He received the Dean’s Prize, BINA’s Excellence Fellowship, the Rector’s Award for outstanding research students, the President’s Fellowship, and the Ministry of Energy’s Fellowship.

Avital Wagner received her BSc and MSc (both summa cum laude) from the Materials Engineering Department at Ben-Gurion University and her MSc under Prof. Nachum Frage involved fabricating and characterizing optically functional YAG ceramics doped with rare-earth elements. Her PhD as an Azrieli Fellow under Dr. Benjamin A. Palmer focuses on the formation and crystallization pathways of biogenic guanine crystals. Avital has extensively used advanced electron microscopy techniques and participated in three experiments performed at synchrotrons in Europe. She also volunteers to teach high school physics to communities in the periphery. She presented her work at many international conferences, published 10 first-author articles in leading scientific journals, and co-authored an additional 15 articles.

The 2024 ICS-Uri Golik Prize winner for an Excellent Graduate Student was awarded to Mr. Yuval Scher of the School of Chemistry, Tel Aviv University, for his pioneering

2024 ICS PRIZE CEREMONY



THE 88TH ANNUAL MEETING OF THE ISRAEL CHEMICAL SOCIETY JERUSALEM FEBRUARY 18-19, 2025

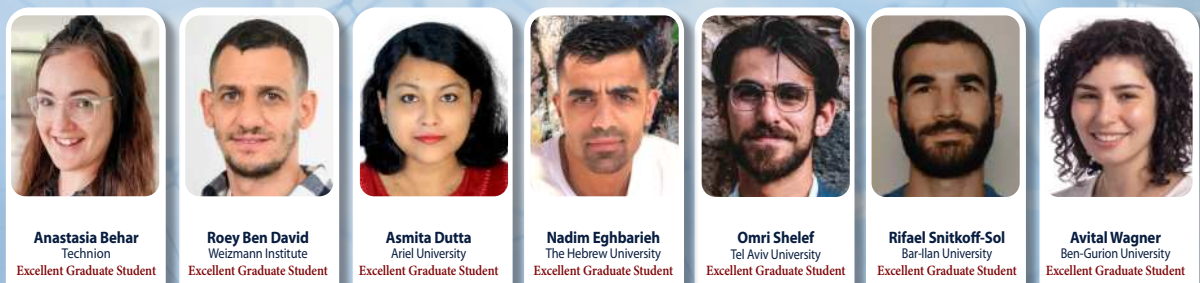
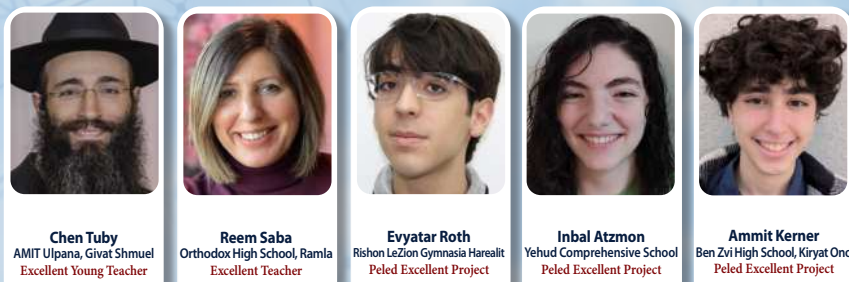
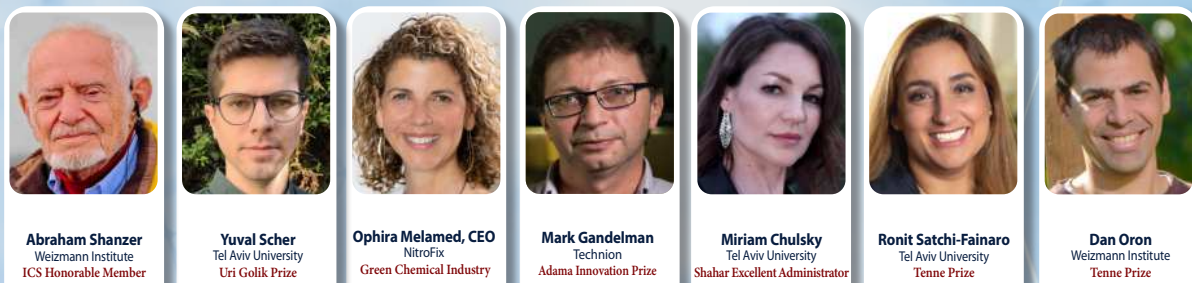
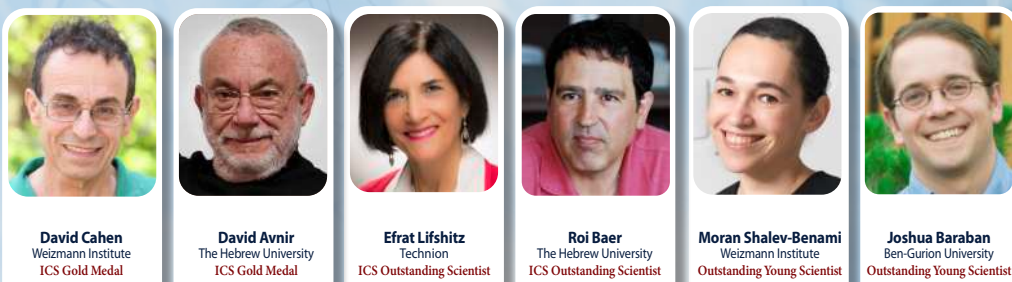


Figure 3. The traditional ICS poster autographed by all 25 prize winners.

contributions to chemical kinetics, single-molecule chemistry, and adsorption-desorption dynamics.

Yuval Scher was born in Tel Aviv in 1992, received his BSc in Chemistry from Tel Aviv University in 2015, and MSc in 2017, magna cum laude, with Prof. Yoram Cohen, studying “Measurement of Transmembranal Exchange Rates by Diffusion NMR Methods.” He measured the transmembranal exchange rate in yeast samples and porcine optic nerves. He succeeded in significantly reducing the FEXSY experiment time without compromising measurement accuracy, with practical implications for human clinical scanners.

His PhD work (2018-2024) with Prof. Shlomi Reuveni in theoretical physical chemistry focused on “Kinetics of Gated Reactions and Sticky Particles.” He borrowed tools from probability and statistical physics to develop and investigate reaction-kinetics theory. For example, in naturally occurring reactions, especially in cellular processes, the reactants do not merely diffuse but constantly interact with the environment and its boundaries. Furthermore, the reactants often possess intricate internal dynamics influencing their reactivity. Similar issues arise when considering transport processes, translational dynamics in the cellular matrix, etc. Yuval developed mathematical tools and models to describe and better understand these phenomena and their effect on reaction kinetics. Another common scenario is the stochastic switch of reactants between reactive and non-reactive states, as is the case for many proteins in our body. Therefore, gating is a central component of enzymatic activity, signal transduction, cellular regulation, and cellular transport. Yuval discovered that gating is not limited to chemical reactions but is also relevant to other dynamic systems, including commodity prices and infected individuals in an epidemic.

Yuval published nine research articles in high-profile journals; in six, he is the first author: *J. Magn. Reson.*, *Phys. Rev. Lett.* (2), *J. Chem. Phys.* (3), *Phys. Rev. Res.*, *bioRxiv*, and *arXiv*. He received the Dean’s Scholarship for excellent PhD students (2022), the Eran and Avital Rabani Award for groundbreaking scientific work in Chemistry (2022), and the David and Paulina Trotsky Foundation Award for PhD Students’ Excellence (2023).

The 2024 Tenne Family Prize in memory of Lea Tenne for Nanoscale Sciences was awarded to Prof. Ronit Satchi-Fainaro of the School of Medicine of Tel Aviv University for rational design and synthesis of novel selective nanoscale delivery systems for targeted drug delivery and immunotherapy; and Prof. Dan Oron of the Faculty of Chemistry of the Weizmann Institute of Science for developing novel optical methods to study nanoscale phenomena, synthesizing nanocrystals and

utilizing them for deciphering the structure-function relation of naturally occurring nanoscale systems.

Ronit Satchi-Fainaro received her B.Pharm from the Hebrew University (1995) and her PhD from the University of London (1999) in polymer chemistry, biochemistry, and cancer nanomedicine. In 2006, following a postdoc at Harvard Medical School, she joined the Department of Physiology and Pharmacology at TAU Faculty of Medicine. In 2015, she became a Full Professor and now serves as Head of the Cancer Research & Nanomedicine Laboratory, Director of Tel Aviv University and its 18-affiliated hospitals’ Cancer Biology Research Center, Director of the TAU Kahn 3D BioPrinting Initiative, and holds the Kurt and Herman Lion Chair in Nanosciences and Nanotechnologies. Her multidisciplinary research laboratory focuses on basic research elucidating the mechanisms underlying the switch from cancer dormancy, leading to the discovery of new molecular targets to interrupt tumor-host interactions. Her pioneering approach is followed by the design of precise nanomedicines to deliver drugs to pathological sites selectively. She has authored over 160 publications, 13 book chapters, edited 2 books, is named inventor on 95 patents, some of which were licensed to pharmaceutical and biotech companies, founded 3 spin-off companies, initiated 2 clinical trials, and has delivered over 600 plenary and invited lectures worldwide. Her 80 graduate students and postdocs are now in academia, industry, hospitals, and government. Ronit was awarded numerous prestigious grants and prizes, among them Fulbright, Rothschild, Alon, JULUDAN, Teva Founders Award, Youdim Prize, Kadar Award, Michael Bruno Memorial Award, Humboldt Foundation Bessel Research Prize, and was elected Fellow of the American Institute of Medical and Biological Engineers (AIMBE), and to the CRS College of Fellows. She was awarded the La Caixa Bank Foundation grant four times, in addition to ERC Consolidator, ERC Advanced, two consecutive PoC, and EIC Transition grants. She serves on the Board of Directors of Teva Ltd.

The 2024 ICS-Adama Prize for Technological Innovation was awarded to Prof. Mark Gandelman of the Schulich Faculty of Chemistry at the Technion for developing innovative technologies for the synthesis of halo-organic compounds.

Mark Gandelman was born in 1972 in Kishinev, Moldova, and immigrated to Israel in 1990. He received his BSc in Chemistry from Tel Aviv University (cum laude, 1995) and a direct track PhD in 2003 from the Weizmann Institute of Science under Prof. David Milstein. He was awarded the Rothschild fellowship for postdoc research at Harvard University with Prof. Eric N. Jacobsen. He then joined the Schulich Faculty of Chemistry at the Technion (2005) and became a full professor in 2020. Mark holds the Abramson Family Chair



Figure 4. Photos from the Award Ceremony of the 88th ICS Meeting. First row from left: ICS Gold Medal: Reshef Tenne, David Cahen, EK; Elad Gross, David Avnir, EK; ICS-Uri Golik Prize: Eran Golik, Moshe Portnoy, Uri Golik, Moshe Cohen, Yuval Scher; Excellent Graduate Students: EK, Anastasia Behar, Efrat Lifshitz; Second row: Excellent Graduate Student: EK, Dan Oron (for Roey Ben David); EK, Asmita Dutta; EK, Nadim Eghbarieh, Elad Gross; EK, Omri Shelef, Moshe Portnoy. Third row: Excellent Graduate Student: EK, Adi Salomon (for Rifael Snitkoff-Sol); EK, Maya Bar Sadan (for Avital Wagner), Tenne Prize: Reshef Tenne, Ronit Satchi-Fainaro, EK, Moshe Portnoy; Reshef Tenne, Dan Oron, EK. Fourth row: ICS-Adama Prize: EK, Mark Gandelman, Efrat Lifshitz, Itsik Bar-Nahum; ICS-Shahar Prize: Dani Shahar, EK, Miri Chulsky, Moshe Portnoy; Cheshnovsky Prize: Dani Shahar, Dorit Taitelbaum, Reem Saba, EK; Cheshnovsky Prize: Dani Shahar, Dorit Taitelbaum, Orit Weinstock (for Chen Tuby), EK. Fifth row: Green Chemical Industry: Ophira Melamed, EK; ICS-Peled Prize: Nechama Peled, Micki Peled, Dorit Taitelbaum, Ilya Olevsko Arad, Amit Kerner, EK, Adi Salomon: Nechama Peled, Micki Peled, Dorit Taitelbaum, Ilya Olevsko Arad, Inbal Atzmon, EK, Adi Salomon; Nechama Peled, Micki Peled, Dorit Taitelbaum, Evyatar Roth, EK. Sixth row: Honorable Member: Avi Shanzer, EK; Dan Oron, Avi Shanzer, EK; ICS Excellent Young Scientist: Dan Oron, Moran Shalev-Benami, EK; Maya Bar Sadan, Joshua Baraban, EK. Seventh row: ICS Excellent Scientist: EK, Efrat Lifshitz, Mark Gandelman; ICS Excellent Scientist: EK, Roi Baer, Uri Banin. Photographs by Dror Sithakol.

in Chemistry. His research program encompasses studies in organometallic, organic, and main-group element chemistry, as well as homogeneous catalysis.

The Gandelman group developed innovative technologies to produce valuable iodo-, chloro-, and bromo-organic materials from readily available, inexpensive carboxylic acids. Production of organic bromides is of special relevance to Israel since the primary bromine consumption (80% of all Br₂ production) goes to produce organic bromides, while Israel is the biggest Br₂ producer. The technologies are metal-free, efficient, robust, and cost-effective.

His group made a groundbreaking impact in organo-fluorine chemistry by developing unprecedented catalytic asymmetric syntheses of organic fluorides. These compounds are highly valuable for pharmaceutical and agrochemical applications. Thanks to technologies developed in the Gandelman labs, the whole families of chiral fluoro-organic materials, including secondary fluoroalkanes, CF₃-substituted alcohols, ethers, and thioethers, can be prepared in a catalytic and stereoselective manner. Based on inexpensive Ni catalysts, the developed technologies are practical and efficient, allowing for the rapid preparation of libraries of novel biologically relevant chiral compounds bearing fluoro-substituent at the desired position.

Gandelman received the Alfred & Yehuda Weissman Award for Excellence in Teaching (2009), the Friedenbergl Prize, Israel Academy of Sciences and Humanities (2011), the Gutwirth Award for Excellence in Research (2012), the Henri Taub Award for Academic Excellence (2012), the Technion Award for Excellence in Teaching (top 4% of lecturers, 2012), the Schulich Prize for Excellence in Enhancing the Understanding of Chemistry (2013), the Klein Prize for Excellence in Research (2014), the Yanai Prize for Enhancing of Academic Education (2014), the David Dodi Ben-Aharon Research Prize (2017), the Hershel Rich Technion Innovation Award (2017), the Sanford Kaplan Prize (2017), and the Joseph and Patricia Vanderslice Lecturer in Organic Chemistry (Boston College, 2017).

The 2024 ICS-Shahar Prize for Excellent Administrative Assistant was awarded to Ms. Miriam Chulsky, a Budget Coordinator and Operations Manager at the School of Chemistry, Tel Aviv University. She will receive the prize for building productive collaborations with stakeholders within and outside the university and for fostering partnerships that enhance operational success.

Miriam (Miri) Chulsky was born in 1978 in Leningrad, USSR (now St. Petersburg), and immigrated to Israel in 1994, where she completed her high school education. Following her military service in 1999, Miri began her academic journey

at Bar-Ilan University, earning a BA with distinction in Social Sciences. Later, she acquired a certificate in accounting management, reflecting her dedication to professional development and excellence. From 2002-2004, Miri worked in youth programs, mentoring, and community engagement initiatives at the Jewish Agency for Israel. In 2005, she joined the Faculty of Engineering at Tel Aviv University as a Procurement Coordinator, where she became a key figure in implementing enterprise resource planning (ERP) systems and optimizing procurement workflows.

In 2014, Miri transitioned to the School of Chemistry at Tel Aviv University as a Budget Coordinator and Operations Manager. In this capacity, she manages the school's budget, including teaching laboratories, service laboratories, and workshops, ensuring close monitoring and control of financial execution. She also oversees procurement processes and ensures compliance with financial regulations, emphasizing efficiency, transparency, and cost-effectiveness. Additionally, Miri provides guidance and support to academic staff in managing research budgets under the university's research authority.

Miri is widely recognized for her exceptional interpersonal skills, her ability to build strong working relationships, and her dedication to fostering a positive, collaborative work environment. She has demonstrated high motivation and a strong commitment to learning and innovation, consistently seeking opportunities to improve processes and introduce creative solutions. Miri has significantly contributed to the School of Chemistry, sharing her experience, knowledge, and skills. Her interpersonal excellence, motivation, and innovative mindset make her an indispensable and highly valued team member.

In 2013, Miri was recognized as an Outstanding Employee at the Faculty of Engineering, and in 2022, she received an Outstanding Employee Award at the School of Chemistry. Miri is also a dedicated family person, married, and a proud mother of two sons.

The 2024 ICS-Dalia Cheshnovsky Prize for excellence in teaching was awarded to two teachers. Ms. Reem Saba of the Orthodox High School, Ramla, received the Excellent Teacher Award for promoting and developing the chemistry profession throughout the country, especially in the Arab sector; developing study units; promoting research laboratories in chemistry; improving chemistry matriculation exams; and training new teachers. Dr. Chen Tuby received the Excellent Young Teacher Award for his contributions to chemistry teaching and the community of chemistry teachers, including developing and promoting innovative teaching

programs and methods in chemistry and the sciences, and assisting new teachers in training to teach chemistry.

The 2024 ICS-Peled Prize for outstanding high-school projects was awarded to Ammit Kerner from the Yitzhak Ben Zvi High School, Kiryat Ono, Inbal Atzmon from the Comprehensive High School, Yehud, and Eviatar Roth from Makif A Gymnasium, Rishon Lezion. Amit Kerner and Inbal Atzmon received the prize for their research on increasing the brightness of plasmonic nanopixels through coupling to fluorescent molecular systems. They conducted their research in Prof. Adi Salomon's laboratory at Bar-Ilan University, with Mr. Ilya Olevsko Arad. Eviatar Roth received the prize for his research on the effect of the amino acid lysine and the phosphate group on the activity of the PL12 peptide in the formation of biosilica. His research was conducted in Prof. Gil Goobes's laboratory with Ms. Jbara Rawan at Bar-Ilan University. The Peled Prize of the ICS is awarded annually in memory of Etan Peled, who perished in 1995 in the Arad disaster.

The 2024 ICS Prize for the Green Chemical Industry was awarded to NitroFix for developing a catalytic electrolyzer that produces green ammonia from water and air at a low voltage. The NitroFix technology, developed by Prof. Ronny Neumann at the Weizmann Institute, focuses on proprietary electrolyzer cell structures, catalysts, and cell components. Reacting water and air within the electrolyzer produces green ammonia at a low voltage, ensuring minimal power consumption. Additionally, the technology incorporates electrolyzers, engineering, and materials science advancements.

Ammonia is a versatile compound essential to various industries, with global annual production reaching approximately 200 million metric tons. The traditional Haber-Bosch process, which uses fossil gas, generates roughly 2.5 tons of CO₂ for every ton of ammonia. Haber-Bosch plants are typically large-scale facilities located near fossil gas sources.

The NitroFix pilot ammonia generator is an electrolyzer connected to renewable energy sources. It requires water and air to function and produces green ammonia, which is stored in a pressurized container. The generator produces ammonia with zero emissions and is suitable for various industries, including agriculture, chemical manufacturing, cosmetics, pharmaceuticals, maritime, and industrial cooling. Ammonia can also be used as a hydrogen carrier, providing a sustainable solution for the hydrogen economy.

NitroFix was selected as one of five cutting-edge companies to join the exclusive H2UB Europe Accelerator in Essen, Germany. The 10-week program began in September and concluded at the Hydrogen Technology Expo in October in

Hamburg. NitroFix was also recognized by the CleanTech Forum Europe as one of the top 50 rising companies in the clean energy sector. Additionally, NitroFix was named one of 20 finalists in the Startup Battlefield 200 at TechCrunch Disrupt. The company was selected by Hello Tomorrow as one of the 2024 Deep Tech Pioneers, recognizing it as a leading deep tech startup.

The 2024 Honorable Member of the ICS was awarded to Prof. Abraham (Avi) Shanzer of the Weizmann Institute of Science. Shanzer received the award for enriching the Israeli chemistry community with creative biomimetic and supramolecular chemistry and for training many successful followers in academia and industry.

Abraham Shanzer was born in 1943 in Israel. He received his MSc in chemistry from Bar-Ilan University (1970) and his Ph.D. from Virginia Polytechnic Institute & State University (1975) in covalent inorganic chemistry. Following postdoc research on organic fluorine chemistry at the same university, he joined the Weizmann Institute (1976) and established a research program on metalloids and organic chemistry. In 1992, he became a Full Professor. He was a visiting Professor at Harvard Medical School, working on biological chemistry (1984-5), and at the Louis Pasteur University in Strasbourg, France, working on coordination chemistry (1992).

His research group focused on molecular recognition in chemical and biological systems. Using naturally occurring bacterial iron binders as model systems, they investigated molecular recognition principles. They synthesized simplified analogs of these complex molecules, which retained their biomimetic ability to bind metals. This work uncovered key principles of molecular recognition, including the effects of rotational symmetry in ring systems, the relative sizes of cavities and metals, the influence of odd-numbered atom spacers between binding sites, and the role of chirality. These discoveries enabled diverse applications across several fields. For example, synthetic siderophore-enhanced dicotyledon growth is relevant to agriculture as it offers chemical alternatives to traditional fertilizers. Fluorescent siderophores enabled real-time monitoring of cell iron uptake, a process relevant to malaria research. Radioactive gallium siderophore derivatives enabled infection tracing in mouse models, advancing diagnostic technologies. Coordination-based supramolecular structures and artificial molecular switches led to innovative gas-detection sensors. Asymmetric bidentate ligands modeled functional active sites of peroxidases. These highly productive studies on ionophore-like molecules also allowed him to collaborate effectively with renowned scientists, including Shneior Lifson, David Samuel, Jacob Sagiv, Israel Rubinstein, Daniella Goldfarb, Yitzhak Hadar,

Avigdor Scherz, Ioav Cabantchik, David Cahen, and Ron Naaman, among others.

Avi's group has published more than 150 research papers in high-profile journals, including *Nature*, *Nature Materials*, *JACS*, and *Angewandte Chemie*, many of which are among the most influential papers in the fields of supramolecular and materials chemistry, garnering hundreds of citations each. Many of his students and postdocs have become leading professors, including Yitzhak Tor (UCSD), Merlin Bruening (Univ Notre Dame), Ellen Moons (Karlstad Univ), David Margulies (Weizmann Institute), Eylon Yavin (Hebrew Univ), Gonen Ashkenasy (Ben Gurion Univ), Michael M. Meijler (Ben Gurion Univ), Galia Maayan (Technion), and Yuri Tulchinsky (Hebrew Univ).

The 2024 ICS Gold Medal was awarded to Prof. David Cahen of the Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, for his pioneering and fundamental contributions to thin-film photovoltaic cells, renewable energy, and biomolecular electronics; and Prof. David Avnir of The Hebrew University of Jerusalem, for pioneering hybrid organic-inorganic materials, including sol-gel functional materials, chiral nano-objects, and an experimental-theoretical approach to quantitative chirality.

David Cahen was born in 1947 in Vught, the Netherlands. After high school, he moved to Israel, obtained his BSc in chemistry and physics from the Hebrew University of Jerusalem (1966-69), MSc (1969-70), and PhD (1970-73) in physical chemistry and materials research at Northwestern University, including a long winter break at Stanford University. David returned to Israel for postdoctoral research on photosynthesis biophysics at the Hebrew University and the Weizmann Institute of Science (WIS). He joined the Weizmann Institute as a faculty member in 1976. Cahen co-pioneered photo-electrochemical solar cells with built-in storage and developed novel experimental means to determine solar cell loss mechanisms. In further solar cell work, he discovered semiconductors' self-healing, surface doping, and molecular control over semiconductor junctions. He focuses on opto(bio)-electronic materials chemistry and physics, emphasizing making such materials sustainable, especially the self-healing of energy materials and proteins as electronic materials. An AVS, MRS, and Helmholtz International fellow and visiting professor at Chiba University, he is also active in energy and sustainability (E&S) research (founding director) and education (organizes and teaches local and international E&S courses; co-edited and wrote *Materials for E&S* textbook), and in science for peace efforts. From 2017-2022, he also ran a research group at Bar-Ilan Univ. He headed the Materials and Interfaces Department. David has published over 400 papers, with over 47,500 citations and an h-index of 109 (Google Scholar).

David Avnir was born in 1947 in a refugee camp in Germany, and his family made aliya in 1949. He received all his education at the Hebrew University, including a PhD under Prof. J. Blum (1977). Following two years of post-doc and one year at Plantex, he joined the Hebrew University (1980) and became a Full Professor in 1988. He served as Head of the Institute of Chemistry. Avnir's diverse research program includes (1) sol-gel materials, incorporating organic and bioorganic molecules within ceramic materials for optics, reactive materials, catalysts, and bioactivity. (2) Fractally disordered materials, including analysis of materials' complexity in terms of scaling properties. Observing the complex, random, and amorphous geometry of natural and synthetic materials, he explained how their surfaces interact with the surrounding world, characterizing, understanding, and predicting their structural correlations with reactivity. (3) Studying chirality and symmetry of molecules and materials on the nanoscale, both computationally and experimentally. He developed a methodology for quantitative evaluation of these structural properties, generalizing chiral imprinting of oxides. (4) Avnir pioneered (in 2002) the molecularly doped bulk metals family. He discovered many traits of these materials, including conductivity, catalytic activity, and the induction of unorthodox properties in metals, such as rendering a metal acidic or basic, forming bioactive metals by enzyme entrapment, and inducing corrosion resistance in iron. Avnir mentored over 65 graduate students and published over 420 papers, garnering over 41,000 citations and an H-index of 86 (Google Scholar). He received the 2004 Kolthoff Award of the Technion, the 2010 ICS Prize for Outstanding Scientist, became a Member of the Academia Europaea (2009), was designated a Distinguished Scientist by the Chinese Academy of Sciences (2018), and received the Lifetime Achievement Award of the International Sol-Gel Society (2013).

David Avnir responded: "It is customary at this stage to thank the master's and doctoral students for their efforts, as the award is for their work. I want to emphasize this point: the instructor proposes a research idea that is often quite vague and general. There is nothing wrong with that, since an idea that has not been implemented is equivalent to a work never being done. It is only thanks to the student's effort, sometimes heroic, to turn an idea into reality that science lays down another brick of knowledge, for which I thank the approximately 70 research students and post-doc researchers who have been with me over the years."

David Cahen responded: "I am very grateful for this recognition. I was attracted to chemistry because I had in 10th grade for one year the one and only really great science teacher at what was a lousy secondary school (classical gymnasium in the very peripheral "deep" South of the Netherlands), in Chemistry (he later went on to write his PhD

thesis on explaining science to the public...). At the Hebrew University, where I did my undergrad in Chemistry & Physics, we had a great scientist running the organic chemistry lab (definitely not my strong side), Yohanan Blum. He must have seen something in me, as otherwise it is a mystery to me how I ever got accepted into some pretty good PhD programs in the USA. I ended up going to Northwestern (with a winter in Stanford to escape the cold). At NU, I had 2 advisors, one in Materials Science and one in Chemistry. The latter told a colleague (who told me some decades later), after I decided to go back to Israel and then to stay there (i.e., I turned down a faculty offer in the US), "I do not understand why someone like Cahen went voluntarily into scientific oblivion." Thank you."

The 2024 ICS Excellent Scientist Prize was awarded to Prof. Efrat Lifshitz of the Schulich Faculty of Chemistry, Technion, for her outstanding research elucidating the electronic structure, optical, and opto-magnetic properties of nano-materials; and Prof. Roi Baer of The Hebrew University of Jerusalem, for his outstanding contributions to theoretical and computational advances in density functional theory.

Efrat Lifshitz was born in 1956 and received her BSc from the Hebrew University (1979) and PhD from the University of Michigan, Ann Arbor, USA (1984). Following postdoctoral research at the Weizmann Institute and the University of Michigan, she joined the Technion in 1990 and became a Full Professor in 2005. Efrat holds the Matwei Gunsbourg Academic Chair and currently serves as the Dean of the Schulich Faculty of Chemistry at the Technion. Efrat pioneered low-dimensional semiconductor solids, applying multifurcating and interdisciplinary approaches that involved the development and preparation of materials, combined with a comprehensive experimental and theoretical investigation of their optical and magneto-optical properties. She explored van der Waals single- and multilayer materials, numerous types of colloidal II-VI and IV-VI semiconductors, and perovskite compounds, deepening understanding of their surfaces, interfaces, trapping/doping, and spin-related effects (dichroism, Rashba, Overhauser) on their photo-physics. She published over 250 high-profile publications and delivered nearly 100 significant lectures at top-tier international meetings. She has also been an active partner in establishing the Nanotechnology and Renewable Energy Centers at the Technion and chaired numerous national and international conferences. Her list of prizes includes the Taub Excellence in Science Award, Technion (2019), the Israel Vacuum Society Excellence Award for Research (2016), the ICS-Tenne Prize (2015), and numerous international lectureship awards. Efrat is an External Senior Fellow at the Freiburg Institute of Advanced Studies (photo by Shlomo Shoham).

Roi Baer was born in Jerusalem in 1961 and earned his BSc in Mathematics and Physics (1982), MSc (1992), and PhD in Chemistry (1996) from the Hebrew University. Following postdoctoral research at UC Berkeley, Baer joined the faculty of the Hebrew University (1998) and became a Full Professor in 2006. He is the director of the Fritz Haber Center for Molecular Dynamics and holds the Ratner Family Chair in Chemistry. Baer is known for developing the concept of range-separated tuning within density functional theory (DFT). This innovative approach significantly broadened DFT's applicability, enabling accurate prediction of diverse molecular properties previously considered beyond its reach, including charge-carrier energies, charge-transfer excitations, Rydberg excitations, the structure of symmetric radical cations, and electric polarizability. This widely adopted technique has been used in thousands of studies and has proven invaluable across a broad spectrum of electronic structure theory. He also pioneered novel stochastic approaches, extending the application of DFT, Green's function perturbation theory, and quantum master equations to large-scale systems. Baer received several awards, including the Josepha and Leonid Olschwang Prize, the Klachky Prize for Advancing the Frontiers of Science, and the Hebrew University's Rector Prize for Outstanding Researcher and Teacher. A dedicated educator, he has mentored numerous students and repeatedly appeared on the Hebrew University's Outstanding Teachers List.

Efrat Lifshitz responded: "I would like to share with you my experience as a scientist over the course of about four decades. I start with the main word – "Thank you for Life" – which gave me the opening to be a scientist, from my natural inclination to the various opportunities on my journey.

The status of a scientist fit me like a glove in my hand. It satisfies my constant curiosity, which was already expressed in my youth. The occasion fulfilled my aspiration to uncover scientific facts and achieve excellence in my actions. The effort and success gave me satisfaction and joy from every discovery and for lasting intellectual stimulation. I had the privilege of being in contact with smart and interesting people, who mutually broadened my horizons and knowledge. I enjoyed mentoring generations of students (almost 60 doctoral students, about 20 master's students, and a similar number of postdoctoral students), and together we went through a challenging journey, learned new fields, and raised them to high levels. Indeed, the experience of success was shared. I'm proud of the next generation that is in respectable jobs around the globe. I am grateful for the privilege of participating in international conferences around the world, for unforgettable experiences, for meeting colleagues abroad, and for creating nourishing collaborations. I also had constructive experiences in professional positions along the way, which enriched me.

As of today, I am continuing this wonderful journey with further plans.

I was asked more than once about my satisfaction with my status, and I answered that if I had to choose a new path, I would choose exactly the one I had experienced. All of this was made possible by my environment. First, the nuclear family substantially supported my ambitions, and later, the Technion established a wonderful institution for scientific development by providing research infrastructure and excellent human resources, creating an atmosphere of action for those who joined the research support organizations.

Finally, I express my deep appreciation to the Israeli Chemical Society for its work across many fields, especially for the annual conferences that bring together Israeli scientists and open the doors to international guests. Special thanks for recognizing the importance of my contributions and for awarding me with a prize today. And to you, the audience, thank you for coming to honor the winners of the awards.”

Roi Baer responded: “It is an honor and a privilege to receive this recognition from the Israel Chemical Society. I want to thank several individuals who have contributed to my journey. I thank my parents, Michael and Malvine Baer. My father instilled in me a love and passion for science from a young age, a gift that has shaped my life and brought me great joy. My wonderful daughters, Ahinoam and Reuth, have provided unwavering love and support, grounding me whenever my work has flown to abstract places and beyond. To my beloved wife, Yael Karshon, a mathematician, who not only sharpens my often mumbled words with precision but, more importantly, embraces my many imperfections with forgiveness and kindness. I thank my close collaborators, Leeor Kronik, Danny Neuhauser, and Eran Rabani, for years of friendship, mutual exploration, loyalty, and support. I owe a deep debt to my past and present students, who have taught me far more than I could have imparted to them. Their invaluable work is the foundation upon which this award is built. I am also indebted to my teachers and close personal friends, Ronnie Kosloff, Hardy Gross, Avinoam Ben-Shaul, Sandy Ruhman, and Micha Asscher. Finally, I wish to acknowledge my co-PIs and scientists, the administrative staff, students of present and past generations, and friends at the Fritz Haber Research Center, as well as the many supporters of the Center, particularly our Beirat members, headed by Professor Gerard Meijer of the Fritz Haber Institute in Berlin. I also wish to thank my colleagues at the Chemistry Institute, who are too numerous to mention individually but together form a group of outstanding scientists and wonderful colleagues and friends.”

The 2024 ICS Excellent Young Scientist Prize was awarded to Dr. Moran Shalev-Benami of the Weizmann Institute of Science, for using structural biology and Cryo-EM to resolve the high-resolution structure and activation mechanisms of complex membrane receptors in the brain in health and disease; and Prof. Joshua Baraban of the Ben-Gurion University of the Negev, for combining experiments and theory to study radical and ionic processes at high temperatures, plasma chemistry, and spectroscopically characterizing transition states.

Moran Shalev-Benami was born in 1982 in Haifa, Israel. She received her BA in molecular biochemistry from the Technion (2006, cum laude), MSc from the Hebrew University in Jerusalem (2008, magna cum laude), and PhD in structural biology of RNA from the Technion, under the supervision of Profs. Timor Baasov and Noam Adir (2013). She then joined Prof. Ada Yonath’s lab at the Weizmann Institute. Since 2015, she has combined her postdoctoral studies in the Yonath group with the group of Prof. Giorgios Skiniotis at the University of Michigan. In 2017, she moved with the Skiniotis group to Stanford University. Moran joined the Weizmann Institute as a Senior Scientist in December 2018. Her research group focuses on the structural biology of membrane proteins, working to decipher the architecture of multiple types of central nervous system receptors. Their discoveries shed light on how the brain regulates appetite and how light modifies brain activity. Moran is a Zuckerman Faculty scholar and holds the Tauro Career Development Chair in Biomedical Research. Her list of awards includes the Klartag Memorial Prize for Excellence in Biochemistry (2013), the Sir Charles Clore Prize for Postdoctoral Fellows (2014), the Weizmann-Abroad Postdoctoral Grant (2015), the Krill Prize (2021), and the Blavatnik Award for Young Scientists (2024).

Joshua Baraban was born in 1983 in New York, NY, USA. He received his BS and MS in Chemistry from Yale University in 2006 with Prof. J. Michael McBride, followed by graduate work at MIT (PhD Physical Chemistry, 2013) on high-resolution gas-phase spectroscopic signatures of isomerization under Prof. Robert W. Field. During his postdoctoral research with G. Barney Ellison and John W. Daily (CU-Boulder), he developed an optically accessible pyrolysis microreactor. In 2017, he joined the Department of Chemistry at Ben-Gurion University of the Negev. His research aims to develop spectroscopic techniques to characterize reactive molecules in their native, exotic environments, such as at high temperatures and in plasmas, thereby revealing fundamental quantum aspects of these species’ chemical properties and dynamics. Inherent in his group’s efforts are the design of novel radical sources and the pursuit of new (often laser-based) methods for their detection. Josh has won several research grants, including ERC Starting, NSF-BSF, Pazy,

Ministry of Energy, and ISF. His list of awards includes the Alon Fellowship for New Faculty (2019), the Krill Prize for Excellence in Scientific Research (2021), and the Toronto Prize for Excellence in Research (2024).

Moran Shalev-Benami responded: “It is my greatest honor to receive the 2024 ICS prize for a young scientist. I want to thank the steering committee, my colleagues, friends, and family for the enormous support over the past year. As all of you know, no science is done alone, so my greatest appreciation goes to the wonderful group of talented students and scientists in my lab who are working day and night to make our scientific dreams come true. Thank you, guys, for never giving up! Our group is a family, a second family, a home, and especially in those difficult times, any of these achievements would not have been possible without you. I also feel privileged to have had the greatest mentors over the years; from each of them, I learned a different aspect of the art of science, and, more importantly, the love of science. So, thank you all for the support, and to the Israel Chemical Society for this great honor.”

Josh Baraban responded: “I thank the ICS and the entire Israeli chemistry community, which has been extremely helpful and welcoming to me since I moved to Israel. I especially thanked my colleagues at BGU, all of whom supported me in one way or another. The credit for the prize goes to my amazing students who performed the research and, last but not least, my family, without whom I would not have been able to do anything.”

Closing ceremony

Prof. Hagay Shpaisman greeted the audience: “Good afternoon, and many thanks for staying until the end of the meeting. I am delighted to close this successful meeting. We reached over 700 participants, 130 lectures, and over 300 posters, a remarkable accomplishment, given that the meeting is not taking place during peaceful times. I am thrilled to pass the baton to the organizers of the 89th ICS meeting, which will take place next February in Tel Aviv.

Before announcing the best poster awards, I’d like to thank all members of the organizing committee, the speakers,

and poster presenters for creating fascinating scientific discussions.

Finally, I am happy to announce the poster awards, all sponsored by BioAnalytics Ltd. We have four awards this year, and I’ll call the awardees in alphabetical order. It is always hard to select four posters out of so many. I cannot name the committee members, but we thank them for their efforts.

“Revealing the DNA Binding Modes of CsoR by EPR Spectroscopy” was presented by Yasmin Igbaria Jaber of Bar-Ilan University, who carried out the work with Lukas Hofmann, Lada Gevorkyan-Airapetov, Yulia Shenberger, and Sharon Ruthstein.

“Ammonia from air: plasma-catalytic NO_x production” was presented by Thierry Slot of the Technion, who carried out the work with Yair Shahaf and David Eisenberg.

“Electrolyte Controlled Regioselective Electro-Reductive Olefin Cross-Coupling” was presented by Daniel Gordon-Levitan of the Weizmann Institute of Science, who carried out the work with Samer Gnaim.

“Universal linear response of the mean first-passage time” was presented by Tommer David Keidar of Tel Aviv University, who carried out the work with Shlomi Reuveni.

Prof. Ehud Keinan concluded the meeting: “At this happy moment, I wish to thank the generous sponsors again: all 8 universities, and the Central Fund for Israel, Jerusalem Development Authority. Special thanks go to the Chairpersons, Hagay Shpaisman and Gerardo Byk, Itsik Bar-Nahum, the ICS Board, our CEO Taly Lidor, who took full responsibility for organizing the event, Dani Shahar of BioAnalytics for his generous support of the poster prizes in addition to sponsoring the Shahar Prize and the teaching excellence prize together with Prof. Ori Chshnovsky. I wish the chairpersons of the 89th meeting, Roey Amir and Yuval Ebenstein, and hope to see you all next February in Tel Aviv.



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