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The Israel Chemist and Chemical Engineer

ICE

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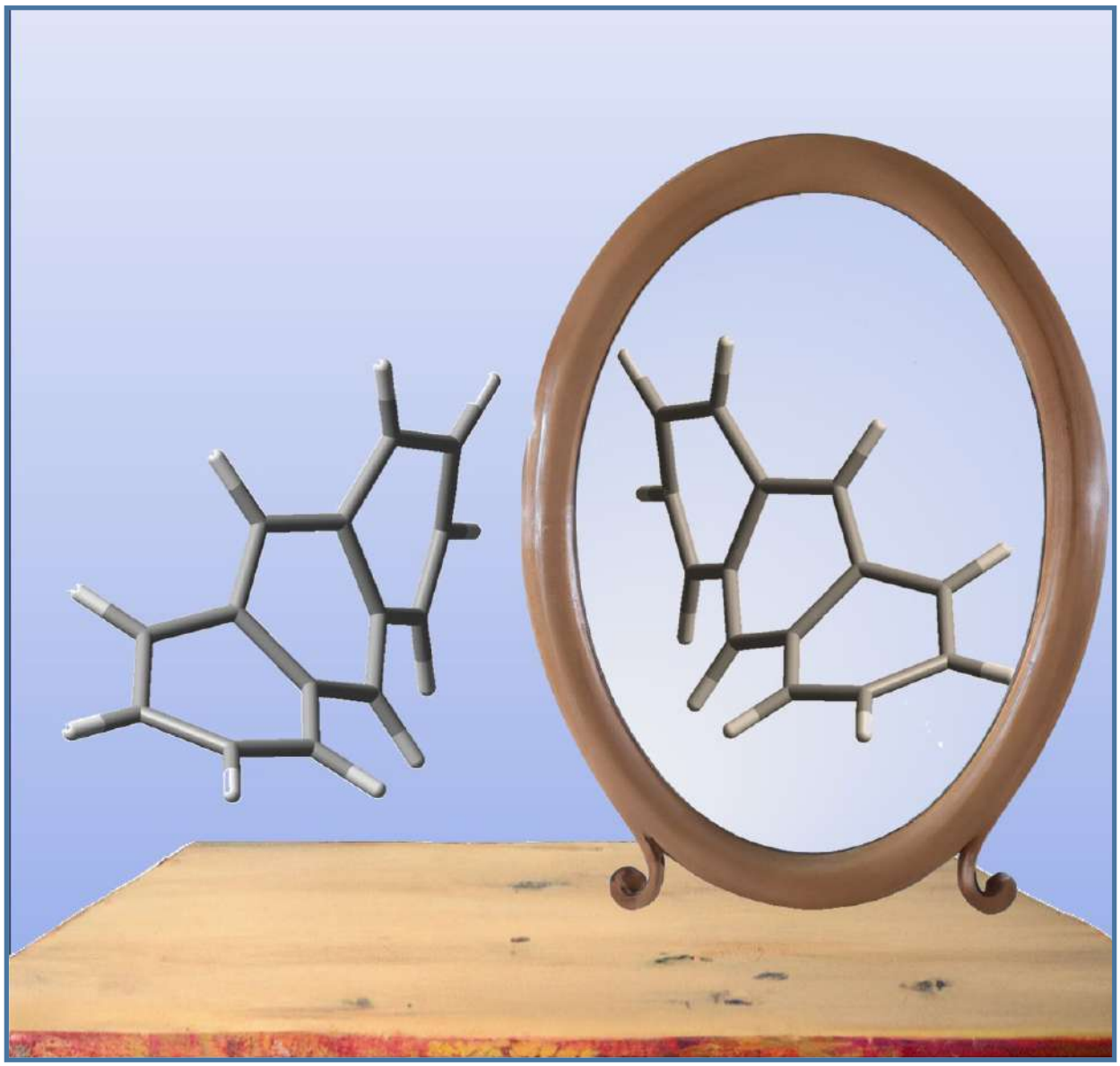

The Israel Chemical Society
(ICS: www.chemistry.org.il)

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Front cover: Ori Gidron "Mirror images"

Dear Readers,

Despite all the major traumatic events in recent months, we welcome you to the tenth 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 five scientific reports on diverse topics from recent ICS prize winners: Aharon Blank, the recipient of the 2022 ICS–Adama Prize for Technological Innovation, has contributed a report on "Magnetic Resonance – from spectroscopic tools to practical technological devices"; Ori Gidron, the recipient of the 2022 ICS Excellent Young Scientist Prize has written on "Aromatic materials – a twisted tale"; Oded Hod, the recipient of the 2022 ICS Tenne Family Prize for Nanoscale Sciences, has contributed an article entitled "Slippery science"; Shlomo Magdassi, the recipient of the 2022 ICS Excellent Scientist Prize, and his coworkers, have written on "Additive manufacturing: from 2D to 4D printing" and Ron Naaman, the recipient of the 2022 ICS Gold Medal, reviews his work on "The chiral-induced spin selectivity effect." I also had the pleasure of interviewing Ron for this issue of the ICE magazine.

Bob Weintraub continues to inform us about the history of science, this time with a timely article entitled "Eugene Rabinowitch (1898-1973): A Voice of Conscience for the Atomic Age."

In this issue, we introduce a new feature on potential careers for chemistry graduates, beginning with Temira Sklarz on "Being a patent attorney (in Israel)."

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,

Before October 7, 2023, we all naively assumed that the COVID-19 pandemic had created the worst possible disruption of our traditional activities. Indeed, the ICS Annual Meeting of 2021 fell victim to the global pandemic, forcing a gap of 2.5 years between the 85th Meeting of February 2020 in Jerusalem and the 86th Meeting of September 2022 in Tel Aviv. Unfortunately, the horrendous massacre of October 7 and the consequential war in Gaza and other fronts forced us to postpone the 87th meeting several times until we finally reduced it to a single day on April 3, 2024 (see my conference report in this issue).

With much hope to get back on track, we scheduled the 88th Annual Meeting for February 18-19, 2025, at the Jerusalem Conference Center, under the leadership of co-chairs Professors Hagay Shpaisman and Gerardo Byk of Bar-Ilan University. We are preparing to host a significant delegation from Taiwan to that event, including ten professors and 20 graduate students.

Nevertheless, we should also remember the many good things that occurred during these tumultuous times. We have signed an agreement with the German Chemical Society on the Richard Willstätter Lectureship. A unique feature of this scientists' exchange program is that the traveling scientists will take with them an excellent graduate student. We plan to apply this unprecedented principle to other exchange programs we are planning now with Taiwan and Japan.

On January 10, 2024, I signed an MOU agreement with the Chemical Society of Japan, and we intend to create another scientist exchange program between Japan and Israel. This agreement adds to five other collaboration agreements we signed earlier with the USA, Germany, Spain, the Netherlands, and the Czech Republic. I hope to sign the seventh agreement with Taiwan soon, supported by an endowment fund of $100,000.

Another exciting development is the establishment of two new Sections of the ICS. The Bioinorganic Chemistry Section under the leadership of Graham de Ruiter, Omer Yehezkeli, and Amir Mizrachi, and the Organic Chemistry Section under the leadership of Doron Pappo, Mark Gandelman, and Elad Shabtai. The establishment of the latter is associated with other exciting news. We have established an international prize and lectureship in memory of the late Prof. Richard Lerner, previous President of The Scripps Research Institute (TSRI). This achievement is a result of a global collaboration, with six of Lerner's friends collectively contributing an endowment of $100,000 to support this annual Prize: Professors Phil Baran, Benjamin F. Cravatt, Jeff W. Kelly, Chi-Huey Wong, and Jin-Quan Yu of TSRI, and Dr. Phillip Frost, former Chairman of Teva Pharmaceutical Industries Ltd. The first Lerner Prize laureate will visit Israel during the annual meeting of the Organic Chemistry Section in May 2025.

I am delighted to introduce the newly elected members of the ICS Executive Board, a group of esteemed professionals who will undoubtedly contribute significantly to the ICS: Roey J. Amir of Tel Aviv University, Itsik Bar-Nahum of Adama, Orna Breuer of Rafael, Ori Gidron of the Hebrew University, Sharon Gazal of Teva, Soliman Khatib of the Tel-Hai College, Dorit Taitelbaum of the Ministry of Education, Michael Meijler (Secretary-General) of Ben Gurion University, David Margulies of the Weizmann Institute, Tomer Zidki (Treasurer) of Ariel University, Igor Rahinov of the Open University, Hagai Shpaisman of Bar-Ilan University, and Ehud Keinan (President) of the Technion. The newly elected Inspection Committee includes Yitzhak Mastai of Bar-Ilan University and Amnon Bar Shir of the Weizmann Institute.

Finally, please help develop the ICE magazine under the leadership of Prof. Arlene Wilson-Gordon, and contribute an article to the ICE on any topic that resonates with you, including popular science, history of science, report on an event, opinions, etc. Your unique perspective is valuable to us. Please, don't hesitate to contact Arlene or me on these matters.

Enjoy your reading,

Ehud Keinan

President, the Israel Chemical Society

Slippery science

Oded Hod
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Abstract:

This is the story of a young man who, while standing at the office doorstep of one of the founding fathers of Israel's chemical physics community, overheard a sentence that shaped his entire career.

Many years ago, at the beginning of this millennium, I was walking around the green paths of the Givat Ram Campus of the Hebrew University of Jerusalem, breathing deeply the clean air, while "shopping" for a PhD position, as coined by my admirable teacher Prof. Ronnie Kosloff. At some point I found myself standing at the doorstep of the great Prof. Raphael Levine. Since my first eye opening quantum mechanics lesson with the late Prof. Victoria Buch, taken at the very same building, I knew that quantum dynamics is what I want to do for a living and that it will never fail to amaze me. This feeling strengthened profoundly when I studied the advanced counterparts of this course, taught skillfully by Prof. Kosloff during a semester-long strike on a sofa in his Jerusalem apartment with his children using him as their living playground, and by Prof. Levine himself. Raphy, if I may use his nickname, was standing in his office, his iconic pipe in his mouth, listening to a student, who seemed to be very convinced by what he had to say. A few minutes later, Raphy interrupted the poor student and said in his calm voice: "When I look in your eyes, I fail to identify the spark and urge to send experimentalists to their laboratories." Now, those who know me can testify that I am a Markovian person, namely, memory is not one of my strong skills. But this specific moment, I will remember till the end of my life. While I knew for a long time that I wanted to be a theoretician, this was the first time when I realized what theory was all about. This very moment shaped my entire independent career, as will soon become clear.

It was Prof. Michael Urbakh, who first introduced me to the field of nanotribology – the science of friction, wear, and lubrication at nanoscale interfaces. I was most amazed when he described the intriguing phenomenon of structural superlubricity, where the atomic lattices of two contacting rigid and flat surfaces form an incommensurate interface that slides with ultralow friction and exhibits friction coefficients lower than 10^{-3}. When he described to me the pioneering 2004 experiment by Dienwiebel *et al.* [1], demonstrating that a twisted nanoscale interface between two graphitic surfaces slides with essentially zero friction (to within experimental error bars), I was truly stunned. What appealed to me the most was the intuitive explanation that he offered, demonstrated

Oded Hod received his BSc from the Hebrew University, Israel, in 1994 and his PhD from Tel-Aviv University, Israel, in 2005. After a postdoctoral fellowship at Rice University, USA, he joined Tel Aviv University in 2008. His research involves computational nanomaterials science including electronic structure, mechanical, electromechanical, and tribological properties, density functional theory, molecular electronics, and electron dynamics and thermodynamics in open quantum systems. Prof. Hod holds the Heinemann Chair of Physical Chemistry, and is an alumnus of the Global Young Academy and the Israel Young Academy. He received Tel-Aviv University's Rector's Award for Excellence in Teaching four times, the 2017 Kadar Family Award for Outstanding Research, the 2022 Tenne Family Prize for Nanoscale Sciences of the Israel Chemical Society, and the 2024 Tel Aviv University Rector's Prize for Teaching Innovation and Creativity.

simply by two egg-box foams that he keeps in his office, each representing the electron density profile associated with the atoms of a given surface (see Figure 1). When stacked in a commensurate configuration, the two foams strongly resist shear stress. This results from the fact that sliding in this case involves the simultaneous crossing of multiple potential energy barriers, all of which are relatively high. However, when twisted into an incommensurate configuration, effective cancellation of lateral forces occurs resulting in a dramatic reduction in the resistance of the foams to slide. In the case of two graphene surfaces sliding across each other a similar picture arises, where the egg box foam peaks are replaced by the electron clouds associated with each atomic site and resistance to sliding occurs due to Pauli repulsions between these electrons as they cross each other.

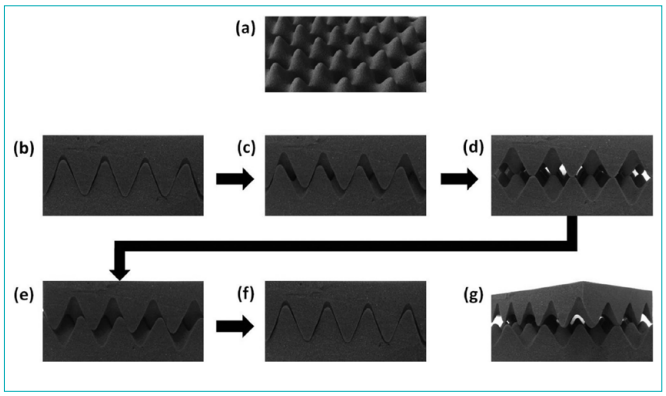

Figure 1. Egg-box foam model for commensurate and incommensurate sliding conditions. (a) Tilted view of a single egg-box lattice. (b)–(f) Relative sliding of two commensurate egg-box foams, where all unit cells cross high sliding barriers simultaneously. (g) A twisted incommensurate interface configuration, where some apexes slide uphill and other slide downhill, resulting in effective cancellation of lateral forces. Adapted with permission from *Phys. Rev. B* **86**, 075444 (2012).

This simple and intuitive explanation made me realize that in such interfaces there is an intimate relation between lattice geometry, interfacial commensurability, and friction. Inspired by this understanding we developed the registry index (RI) – a simple and intuitive geometric measure, based on projected overlaps of circles associated with atomic positions in adjacent surfaces, which quantifies the degree of commensurability of interfacing lattices [2-4]. Using this simple geometric tool, we were able to fully reproduce, down to fine details, not only the sliding potential energy surface, but also the measured twist angle dependence of the friction force at homogeneous nanoscale graphitic interfaces in both the high and ultralow friction regimes (see Figure. 2) [5].

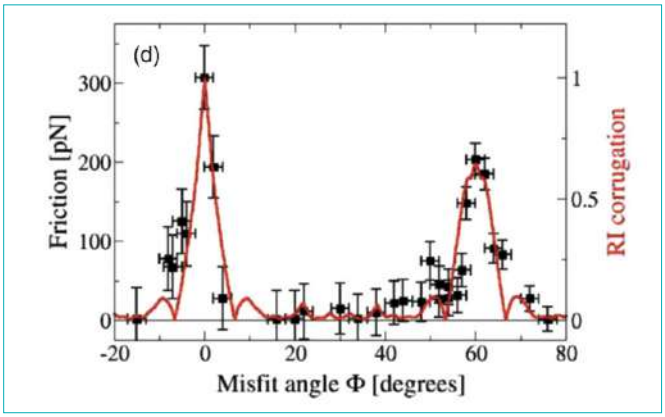

Figure 2. Measured friction (black circles; left axis) and corrugation of the registry index landscape (red line; right axis) as a function of the twist (misfit) angle for a hexagonal multilayer graphene flake sliding along the armchair direction of a graphite surface. Adapted with permission from *Phys. Rev. B* **86**, 075444 (2012).

The 2004 experiment by Dienwiebel *et al.* [1] generated great enthusiasm for the utilization of graphitic flakes to achieve large-scale superlubricity. Naively, one could suggest covering any two surfaces with a sufficiently thick graphite layer that will buffer the contact from the microscopic corrugation of the underlying substrates. Introducing graphitic flakes of random orientations into the flat interface would then result in multiple nanoscale junctions, most of which forming incommensurate contacts. This multi-nanocontact setup could then lead to macroscopic superlubricity, while avoiding the undesirable effects of large-scale surface elasticity. Unfortunately, this beautiful and simple idea was refuted by Filippov *et al.* in 2008, who showed that dynamical reorientation of the flakes aligns them at the lowest energy stacking which unfortunately is commensurate, such that the interface slides along the most highly corrugated potential energy path [6].

A few years later, the understanding that commensurability and friction are intimately related in layered material contacts led us to suggest a simple remedy to this problem [7]. Given that at the aligned configuration the homogeneous graphitic contact is commensurate, all that had to be done is to replace one of the contacting graphene surfaces by a similar surface of a different lattice parameter, thus forming a heterogeneous contact. The natural choice was hexagonal boron nitride (*h*-BN), which has the same hexagonal structure as graphene, but with boron and nitrogen atoms replacing each pair of adjacent carbon atoms. Since the two materials have a lattice mismatch of 1.8%, even at the aligned configuration, where the lattice vectors of the two surfaces are parallel to each other, an incommensurate flat contact is formed. In terms of the macroscopic analogy, one can imagine two egg-box foams

of different periodicity such that, even when aligned, they cannot be appropriately interlocked. In such a case, therefore, friction is expected to be small. To prove that this idea is feasible, we used the RI approach and showed that, indeed, as the area of the heterogeneous contact grows beyond the moiré supercell dimensions the corrugation of the sliding energy profile remains low regardless of the twist angle (see Figure 3). This suggested that heterogeneous contacts of layered materials should demonstrate superlubric behavior that is robust against dynamical twisting.

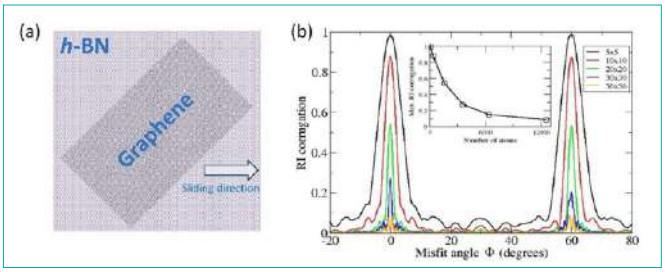

Figure 3. Effect of flake size and twist (misfit) angle on the corrugation of the sliding RI surface of the heterogeneous graphene/*h*-BN interface. (a) Schematic representation of a square graphene flake on top of an *h*-BN layer with a misfit angle of 45°. The sliding direction is marked by the white arrow. (b) Maximal variations of the RI calculated along linear paths in the sliding direction as a function of interlayer misfit angle. (Inset) Maximal RI corrugation as a function of flake size (number of atoms in the flake). The different diagrams presented in panel (b) are normalized to the size of the relevant graphene flake, such that a maximal RI corrugation of 1 is obtained for a strained graphene flake consisting of the same number of atoms and geometry having no lattice mismatch with the underlying *h*-BN layer. Adapted from *J. Phys. Chem. Lett.* **4**, 115–120 (2013) (published under CC-BY 4.0).

After giving a talk on this topic at a conference held in Beijing, China, Prof. Urbakh asked me to deliver a colloquium for the group of Prof. Quanshui Zheng of Tsinghua University. About two thirds into the colloquium, when I presented the idea of robust superlubricity, Prof. Zheng stopped me and started interrogating me regarding this specific prediction. About five minutes later, he halted and said: "I am going to measure this!" Well, this indeed is a decisive moment in the life of every theoretician. Someone is actually going to measure my prediction, I thought. What if it won't work? Nonetheless, I finally had the opportunity to drive experimentalists to perform experiments, as Prof. Levine taught me, unwittingly, many years before.

A couple of years later and many sleepless nights of Prof. Zheng's students, our prediction was finally verified [8-12]. Bravely, they considered layered material junctions of contact area, which is ~9,000,000 times larger than the contact area studied in the canonical 2004 experiment. Yet, while the homogeneous graphitic contact presented very large frictional anisotropy, the heterogeneous system exhibited ultralow friction and superlubric behavior even for the aligned configuration (see Figure 4). Notably, these experiments were performed at room temperature and under ambient conditions, namely in the presence of surface contaminants. A simple run-in process was further shown to remove intercalated species from the sliding interface, pushing the system even further into the superlubric regime. Following that, several other experimental demonstrations of robust structural superlubricity in microscale heterogeneous interfaces have been presented in the literature, further demonstrating the generality of the effect [13].

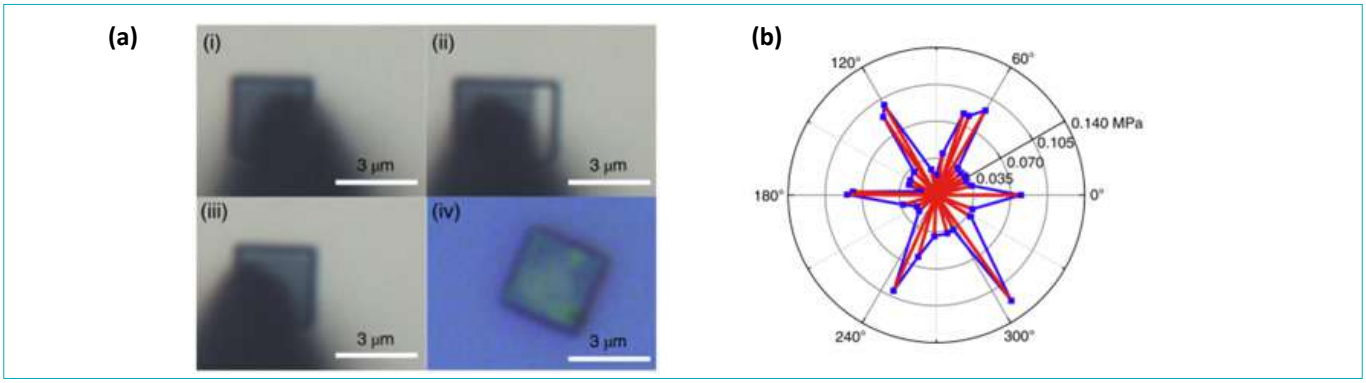

Figure 4. Experimental demonstration of robust superlubricity in a graphene/*h*-BN interface. (a) Optical images of a graphite/*h*-BN heterostructure fabrication. (i) Attachment of a tungsten probe to the SiO_2 cap of an HOPG mesa. (ii) Tungsten probe shearing of a graphitic mesa results in the drag of the mesa's top section. (iii) Self-retraction motion exhibited by the dragged graphitic flake atop the lower graphite mesa section on release from the tungsten probe. (iv) Transfer of the graphitic flake onto the *h*-BN surface. (b) Dependence of the frictional stress on the twist angle between the monocrystalline graphitic flake and the *h*-BN substrate measured under ambient conditions (temperature of 22 ± 1 °C and relative humidity of 29 ± 3%). The sliding velocity was set to 200 nm/s and the normal load was kept at 19.7 μN. Adapted with permission from *Nat. Mater.* **17**, 894–899 (2018).

By harnessing some scientific intuition, a simple idea, basic geometric considerations, and a lot of luck we were therefore able to encourage experimentalists to perform groundbreaking studies that pushed the limits of structural superlubricity orders of magnitude forward. Following that, the powerful RI tool that we developed was extended to describe other homogeneous and heterogeneous layered material interfaces [7,14], curved contacts [3,15], as well as electric polarization profiles in non-centrosymmetrically stacked layered material interfaces [16]. Nonetheless, the RI approach assumes rigid interfaces, thus neglecting edge pinning effects and elastic considerations that may become vital to understand the mechanisms underlying friction in large-scale interfaces, especially when moiré superstructures emerge. To address these important issues, we had to resort to another computational resource, namely molecular dynamic simulations based on classical force-fields. Here, the story begins again with a twist, but this time of nanotubes. As kids in the small city of Rehovot, we used to play a little game called "קוצים" ("thorns"), where we twisted the skin on our friends' arms, giving them a prickly feeling. Many years later, Prof. Ernesto Joselevich of the Weizmann Institute of Science, who was my teaching assistant back in the previous millennium, had a habit of playing "thorns" with nanotubes. Using an ingenious experimental setup, he was able to twist the outer shell of multi-walled nanotubes and measure their mechanical and electronic response [17-18]. Being a young faculty member at the School of Chemistry of Tel Aviv University, I was quite surprised when Ernesto approached me asking whether I can perform simulations that will help provide an atomistic rationalization of the intriguing experimental results that he has obtained for twisted boron nitride nanotubes (BNNTs). With enthusiasm I approached my then graduate student, Dr. Itai Leven, and asked him to find an appropriate force-field for BNNTs. After a couple of days of literature search Itai came back with good news and bad news. The good news was that there exists a dedicated force-field, developed by Kolmogorov and Crespi, that appropriately accounts for the anisotropic nature of layered materials and can treat both the sliding and binding physics in layered interfaces [19-20]. The bad news was that this force-field was never parameterized for any interface, apart from bilayer graphene. This, in fact, turned out to be even better news, as it provided us with a whole new playground of opportunities for the development and parameterization of force-fields, dedicated to layered material interfaces, in the context of nano-tribology. After nearly ten years of work in collaboration with Michael, Prof. Leeor Kronik of the Weizmann Institute of Science, and several very talented students and post-doctoral fellows, our anisotropic interlayer potentials are currently publicly available for a variety of homogeneous and heterogeneous layered material interfaces composed of graphene, *h*-BN, and several prominent members of the vast transition-metal dichalcogenides family [21-26].

These powerful simulation tools that provide a desirable compromise between physical accuracy and computational burden, allowed us to study a variety of interesting problems, and rationalize intriguing experimental findings. These include the faceting of multiwalled nanotubes [27-28]; frictional mechanisms of grain boundaries in polycrystalline surfaces [29-32]; bulk penetration of surface perturbations [33]; serpent-like motion, peeling, and direct growth of GNRs on semi-conducting surfaces [34-36]; surface reconstruction in marginally twisted layered interfaces leading to the emergence of ferroelectricity [37], and multi-contact superlubric interfaces of graphullerene and graphene [P. Ying, O. Hod, and M. Urbakh, Superlubric Graphullerene *Nano Lett.* **24**, 10599–10604 (2024)].

Beyond unveiling the mechanisms that underly existing experimental results, the developed force fields also have predictive power. This was demonstrated for the case of twist angle dependent interlayer heat transport through layered interfaces, which was predicted and explained computationally [38] prior to its experimental exploration [39]. It was also shown for the prediction of negative differential friction coefficients over moiré superstructures and grain boundaries in polycrystalline layered material surfaces [29-30, 40]. Here, a unique mechanism of energy dissipation at corrugated grain boundaries was identified, where a vertical snap-through motion of grain boundary protrusions results in enhanced energy dissipation into lattice phonon modes. The application of external normal load suppresses this out-of-plane motion and reduces the energy barrier associated with the snap-through process, resulting in a smoother transition and lower frictional energy loss. This prediction was recently verified experimentally for the friction over grain boundaries of polycrystalline graphene grown atop a Pt(111) surface [41].

Apart from grain boundaries, an additional source of friction that emerges with increasing contact area are surface defects, e.g. lattice vacancies, that may induce interlayer covalent bonding. This scenario eliminates the main computational advantage of treating anisotropic layered interfaces, namely the ability to distinctly distinguish between the description of intralayer and interlayer interactions. This, in turn, makes the development of traditional reactive anisotropic potentials a highly challenging task. A viable alternative that became available only in recent years can be found in machine learning potentials (MLPs). The main conceptual disadvantage of this methodology is that it lacks an explicit mathematical expression to describe the various interactions based on physical considerations. This blurs the

fundamental understanding of how individual interatomic interactions influence the overall properties and dynamical behavior of the system. Furthermore, since they do not utilize simple dedicated interaction expressions based on physical intuition, MLPs require extensive parameter sets and parameterization procedures, making them typically much more computationally demanding. Nonetheless, these apparent disadvantages mark also the main strengths of this approach as, given a sufficient large training set, often based on first-principles calculations and a large enough parameter set, the same machinery can, in principle, handle any scenario on the same footing, regardless of its complexity. Therefore, in the case of reactive sliding, where the distinction between intra- and inter-layer interactions becomes ill defined, we have recently adopted MLPs as a useful alternative to traditional physically motivated anisotropic force fields. This allows us to characterize the effects of structural defects and interlayer covalent bonding on the frictional properties of graphitic interfaces (see Figure 5 and P. Ying, X. Gao, A. Natan, M. Urbakh, and O. Hod, "Chemifriction and Superlubricity: Friends or Foes?", submitted (2024), and P. Ying, A. Natan, O. Hod, and M. Urbakh, "Effect of Interlayer Bonding on Superlubric Sliding of Graphene Contacts: A Machine-Learning Potential Study", *ACS Nano* **18**, 10133-10141 (2024)).

As discussed above, the scaling-up of robust structural superlubricity opens the door for novel friction-free and wear-less technologies. Nonetheless, friction is often unjustly associated only with negative implications. In a recent study, we have been able to demonstrate how friction at the molecular level [42] can be harnessed to achieve enantio-separation [43-44]. Chiral molecules are molecules whose mirror image cannot be superimposed on their original structure, just like the palm of a human hand (χειρ (kheir) in Greek). The two mirror image structures are called enantiomers. Notably, numerous bioactive molecules in living organisms are characterized by homo-chirality, e.g. chiral receptor molecules of a well-defined handedness. As a result, different enantiomers of chiral medical consumables may have different medicinal activity, to the point where one enantiomer may be of therapeutic benefit, whereas its mirror image can be toxic or harmful at the same dosage. Hence, the separation of enantiomers from of a racemic mixture is an important chemical process with vast pharmaceutical and economic implications. Traditional enantio-separation approaches are based on column chromatography technologies, where a dedicated chiral substrate selectively absorbs a given enantiomer over its counterpart. While this technology is very effective, it requires the development of specific chiral substrates for any given target molecule and is not environmentally friendly, considering the waste that obsolete substrates produce. Hence, the development of more generic, economically efficient, and green approaches is desirable. Here, friction may come into play.

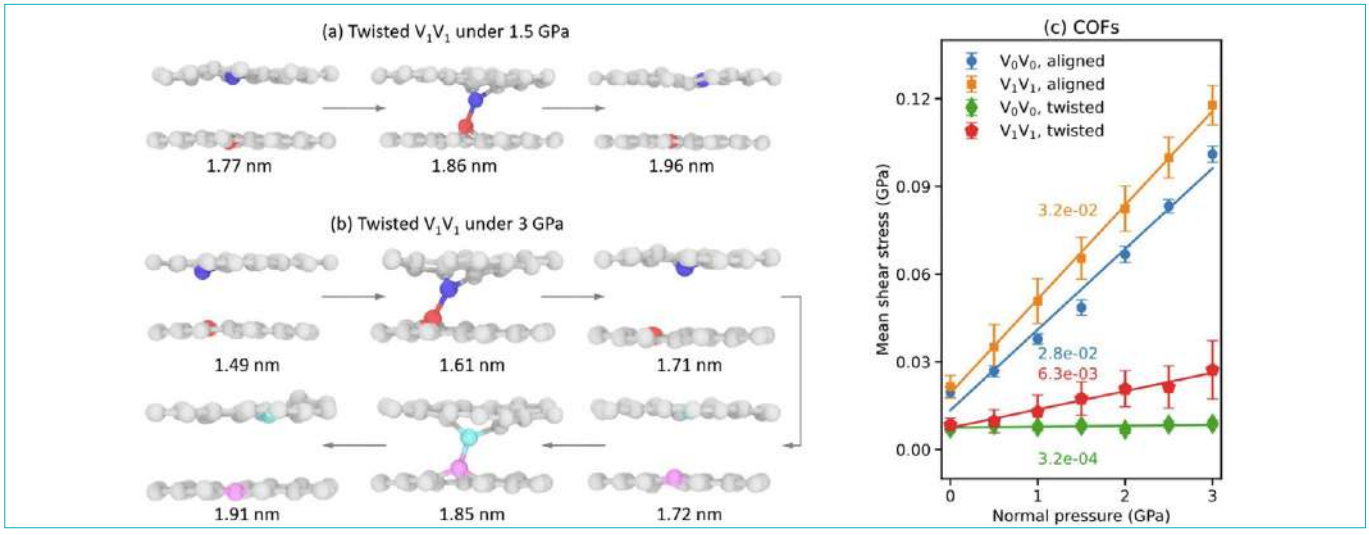

Figure 5. Results of MLP dynamical friction simulations of a double-vacancy defected graphene interface. (a) Snapshots from a twisted interface simulation trajectory, performed at room temperature and under an external pressure of 1.5 GPa, demonstrating a single bond formation and rupture event during sliding. (b) Same as panel (a) but under an external pressure of 3 GPa, where the system exhibits two consecutive events of bond formation and rupture. Only atoms in the vicinity of the defects are presented and atoms involved in interlayer bonding are highlighted. Lateral displacements are annotated below each snapshot. (c) Mean shear stress (averaged over a displacement of 5.2 nm of the ensemble-averaged trace) as a function of normal pressure for the aligned (orange) and twisted (red) double-defect interfaces. The defect density for the aligned and twisted interfaces are 0.24% and 0.34%, respectively. Results of the corresponding pristine interfaces are presented in blue and green, respectively. Adapted from *ACS Nano* **18**, 10133–10141 (2024) under CC-BY 4.0 license.

Imagine a soccer ball dropped on the surface of an ice-skating rink. The ball will bounce straight up regardless of if it was spinning about its center-of-mass or not. Should the ball be dropped over an asphalt surface, though, its spinning sense would dictate whether it would bounce forwards or backwards, due to the friction force acting at the contact region. By replacing the ball with a chiral molecule, whose rotational sense can be separately controlled for each of its enantiomers using an appropriate sequence of external electromagnetic pulses, frictional spatial enantio-separation may be achieved [43-44]. Since friction is a generic phenomenon, no specific substrate is required, and the only molecule-specific element in the separation procedure might be the design of the electromagnetic pulse train. Furthermore, since no adsorption is involved in the process, waste production and ecological signature are expected to considerably reduced.

At this point, you may have noticed that despite mentioning that I realized early on that quantum dynamics is what I want to do for a living, until now all I told you about revolves around classical mechanics. What I failed to disclose thus far is that many of the ideas that I mentioned actually emerged from my interest in, and work on, electron dynamics in open quantum systems. Being a PhD student at Tel Aviv University I had the privilege to be mentored by Prof. Eran Rabani and Prof. Roi Baer, and to take advanced courses in "Chemical Dynamics in Condensed Phases" by Prof. Abraham Nitzan, "Quantum Scattering Theory" by the late Prof. Abraham Ben-Reuven, and "Chemical Applications of Path Integrals" by Prof. Mordechai Bixon. Being in the department founded by the great Prof. Joshua Jortner and influenced by the spirit of these quantum dynamics founders and giants ignited my passion for the field of molecular electronics. I truly fell in love with the concept of being able to control electronic flow through molecular constrictions, design the junction properties via the chemical structure of the scattering center, and suggest new molecular scale electronic devices with novel functionalities.

My initial steps in this field were taken already during my PhD studies, where we predicted that one can use the Aharonov-Bohm effect to switch the conductance through a molecular ring by applying an external traversal magnetic field [45-51]. While this was well known for mesoscopic rings, because the response of the system is proportional to the magnetic flux it was widely accepted that molecular rings cannot exhibit such an effect with feasible magnetic fields, due to their small enclosed area. We have been able to show that while the full Aharonov-Bohm period in molecular rings remains way out of reach of present experimentally accessible magnetic fields, its sinusoidal shape can be altered by controlling the coupling between the circular molecule and the contacting metallic leads. Taking advantage of coherent interference effects then allowed us to achieve sharp current response at low magnetic fields. This work served as a basis for later collaborative studies with Prof. Nitzan on the emergence of circular currents in molecular rings of various topologies [52-54].

I did not neglect my passion for quantum mechanics and dynamics during my post-doctoral term with Prof. Gustavo E. Scuseria at Rice University, Houston, Texas. There, I developed, in collaboration with Prof. Juan E. Peralta, a first-principles divide and conquer approach to study steady-state current characteristics of elongated molecular junctions [55]. We further developed a time-domain time-dependent density functional theory (TDDFT) code, within the Gaussian suite of programs, which allowed us to study spin dynamics in molecular magnets [56].

After establishing my own group, I set out on a quest to develop a theory and a computational scheme for the simulation of electron dynamics in open quantum systems, with emphasis on molecular electronics scenarios. The goal was to formulate a methodology that is theoretically simple, physically intuitive, and easy to implement, especially within the realm of TDDFT. I identified all three criteria in a method proposed separately by Sánchez et al. [57] and Subotnik et al. [58] that couples a finite model system, consisting of two explicit lead models and an extended molecule section (composed of the molecule and its adjacent lead sections) to external Fermionic leads of different thermal equilibria states, using the following augmented single-particle density-matrix-based Liouville–von Neumann (LvN) equation of motion (EOM):

$$\frac{d\boldsymbol{\rho}(t)}{dt} = -\frac{i}{\hbar}[\boldsymbol{H}(t), \boldsymbol{\rho}(t)] - \Gamma \begin{pmatrix} \boldsymbol{\rho}_L - \boldsymbol{\rho}_L^0 & \mathbf{0} & \boldsymbol{\rho}_{L,R} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boldsymbol{\rho}_{R,L} & \mathbf{0} & \boldsymbol{\rho}_R - \boldsymbol{\rho}_R^0 \end{pmatrix}, \quad (1)$$

where $\hbar$ is the reduced Plank constant and $i \equiv \sqrt{(-1)}$. Here, the first term on the right-hand side is the standard propagator of the LvN EOM for a closed system, where $\boldsymbol{\rho(t)}$ is the single-particle density matrix, which in the block matrix representation has the following form:

$$\boldsymbol{\rho}(t) = \begin{pmatrix} \boldsymbol{\rho}_L & \boldsymbol{\rho}_{L,EM} & \boldsymbol{\rho}_{L,R} \\ \boldsymbol{\rho}_{EM,L} & \boldsymbol{\rho}_{EM} & \boldsymbol{\rho}_{EM,R} \\ \boldsymbol{\rho}_{R,L} & \boldsymbol{\rho}_{R,EM} & \boldsymbol{\rho}_R \end{pmatrix}, \quad (2)$$

and

$$\boldsymbol{H}(t) = \begin{pmatrix} \boldsymbol{H}_L & \boldsymbol{V}_{L,EM} & \mathbf{0} \\ \boldsymbol{V}_{EM,L} & \boldsymbol{H}_{EM} & \boldsymbol{V}_{EM,R} \\ \mathbf{0} & \boldsymbol{V}_{R,EM} & \boldsymbol{H}_R \end{pmatrix} \quad (3)$$

is the single particle Hamiltonian in the same block matrix representation. Here, ρ_i and H_i are the density and Hamiltonian matrix representation blocks of the left *(i=L)* and right *(i=R)* lead models, and the extended molecule *(i=EM)* section, respectively, and $\boldsymbol{\rho}_{i,j}$ and $\boldsymbol{V}_{i,j}$ are the corresponding coherences and coupling blocks. For simplicity, direct lead-lead couplings are neglected. The second term on the right-hand side of Eq. (1) drives the lead state occupations towards Fermi-Dirac equilibrium distributions at a rate Γ, which can be determined from first principles [59], via diagonal block matrices $(\boldsymbol{\rho}^0_{i=L,R})_{k,k'} = \delta_{k,k'}\left[1+e^{(\varepsilon^i_k-\mu_i)/(k_BT_i)}\right]^{-1}$, where $\{\varepsilon^i_k\}$ are the sets of eigenenergies of the left and right lead sections μ_i and T_i are the target chemical potentials and electronic temperatures of the leads, respectively, and k_B is the Boltzmann constant. This term effectively couples the left and right leads of the finite system, which are explicitly modeled, to two implicit reservoirs at different equilibria states, thus inducing dynamical current flow through the system.

I found the method to be so elegant and simple that immediately after reading the papers I implemented it for a tight-binding model. I was very happy to find out that it works extremely well in the case where the leads and the molecule are strongly coupled. However, in the weak-coupling limit, which is very common in the field of molecular electronics, it failed badly. Determined to remedy this, I joined forces with Leeor, and together with our joint student, Dr. Tamar Zelovich, we set out to solve the problem. Over a period of a few months, we explored many ideas without success, and frustration led us to search for alternatives.

It may seem unrelated at first, but in my mail browser I have way too many folders, one of them though is a little treasure chest, which I call "ideas". This is a folder where I file emails that I send to myself with ideas that come up every now and then and I have no time to explore. While we were racking our brains trying to find out why the density-matrix approach fails to work at the most interesting and relevant limit, I sent myself several notes on ideas that I thought we should try. Unfortunately (or maybe fortunately), I did not have time to explore these ideas until one day, I and my daughter were ill and stayed at home. Suddenly, I found myself free of duties and my ideas mail folder was calling for me. I coded the first idea, namely the periodic resetting of the finite reservoir occupations and coherences every few time steps, and it failed. I then implemented the second idea, which involved an additional periodic resetting of the reservoir-system coherence blocks, and finally – it worked! After the initial thrill, I was still unsatisfied with this solution, which was based on an unphysical numerical trick. However, it provided very important insights regarding the missing ingredient in the original approach. By adding damping also to the reservoir-system coherence blocks, in the following manner:

$$\frac{d\boldsymbol{\rho}(t)}{dt} = -\frac{i}{\hbar}[\boldsymbol{H}(t),\boldsymbol{\rho}(t)] - \Gamma\begin{pmatrix}\boldsymbol{\rho}_L-\boldsymbol{\rho}_L^0 & \boldsymbol{\rho}_{L,EM} & \boldsymbol{\rho}_{L,R}\\ \boldsymbol{\rho}_{EM,L} & \mathbf{0} & \boldsymbol{\rho}_{EM,R}\\ \boldsymbol{\rho}_{R,L} & \boldsymbol{\rho}_{R,EM} & \boldsymbol{\rho}_R-\boldsymbol{\rho}_R^0\end{pmatrix}, \tag{4}$$

everything finally worked like a charm. I was so excited that once I recovered from my illness, I rushed into Abraham Nitzan's office and showed him the result. After a few seconds he answered: "Of course you have to damp the coherence matrix blocks, and by the way – you are missing a factor of 2." He pointed me to his "Chemical Dynamics in Condensed Phases" book, which is based on his courses that I took ages before, and showed me the proof for the missing factor of 2. Luckily, I failed to understand the proof, so I came up with an alternative heuristic derivation (based on the substitution of a non-Hermitian Hamiltonian within the LvN EOM) of what

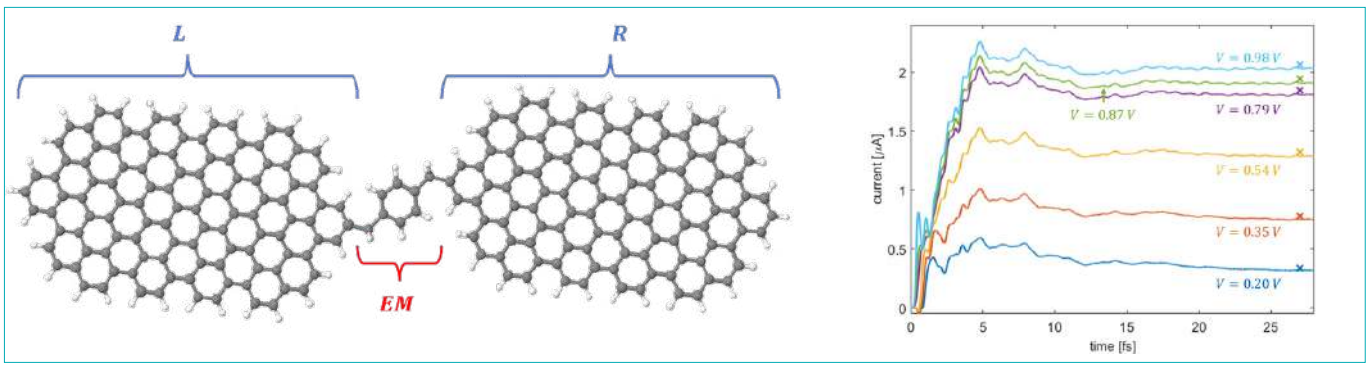

Figure 6. Demonstration of a TDDFT transport simulation using the DLvN approach. (a) Real-space formal partitioning of a molecular junction model composed of two finite graphene nanoribbons bridged by a benzene molecule, into left (L) and right (R) lead sections and an extended molecule (EM) region. (b) Time-dependent current calculated for the GNR junction shown in panel (a). Different bias voltages are considered (all values are marked in the figure) with reservoir electronic temperatures of $T_L = T_R = 315.7$ K and a driving rate of $\hbar\Gamma = 1.09$ eV. The colored × marks designate the corresponding steady-state currents. Adapted with permission from *J. Chem. Theory Comput.* **19**, 7496–7504 (2023).

is now termed the driven Liouville von Neumann (DLvN) EOM [60-61]:

$$\frac{d\boldsymbol{\rho}(t)}{dt} = -\frac{i}{\hbar}[\boldsymbol{H}(t), \boldsymbol{\rho}(t)] - \Gamma \begin{pmatrix} \boldsymbol{\rho}_L - \boldsymbol{\rho}_L^0 & \frac{1}{2}\boldsymbol{\rho}_{L,EM} & \boldsymbol{\rho}_{L,R} \\ \frac{1}{2}\boldsymbol{\rho}_{EM,L} & 0 & \frac{1}{2}\boldsymbol{\rho}_{EM,R} \\ \boldsymbol{\rho}_{R,L} & \frac{1}{2}\boldsymbol{\rho}_{R,EM} & \boldsymbol{\rho}_R - \boldsymbol{\rho}_R^0 \end{pmatrix}. \quad (5)$$

It was only after deriving this EOM, when I realized that at the doorstep of my office there is an engraved tile designed by the late Prof. Ben-Reuven, who was the former resident of this office, with an equation that is reminiscent of the DLvN EOM. At this point I was also able to identify a misprint in the engraved equation, which you are more than welcome to explore next time you visit me.

The application of a simple unitary transformation to the EOM, termed the site-to-state transformation, allowed us to extend the applicability of the approach beyond phenomenological models to atomistic descriptions of realistic molecular junctions [59, 62-65]. This, in turn, paved the way for the application of the approach within the realm of TDDFT (see Figure. 6) [66]. Furthermore, the approach was shown to constitute an efficient numerical scheme to study the thermodynamic properties of open quantum systems [67-68]. I note in passing that the driving term appearing in Eq. (5) and the site-to-state transformation served as inspiration for the application of remote thermal baths and for the analyses of results obtained in some of our classical molecular dynamics simulations, such as the study of heat transport through twisted layered material interfaces [38].

Very recently, another related circle was closed, when I was approached by Prof. Harry Anderson of the University of Oxford, a world expert in the synthesis of macrocyclic molecules, regarding the possibility of measuring Aharonov-Bohm current switching in molecular rings. It is hard to describe the thrill that I experienced while realizing that my old studies with Profs. Rabani, Baer, and Nitzan triggered the interest of a leading chemist, such as Prof. Anderson. These days, we are finalizing our first manuscript on the subject, demonstrating that the experimental realization of our predictions of molecular Aharonov-Bohm interferometry is on the verge of being within our reach with present technologies.

Developing theoretical tools and computational methodologies that enable the prediction of novel physical phenomena, which eventually leads to experimental efforts towards their verification and utilization, is for me a great privilege. It fully complies with the important philosophical lesson that I unintentionally learned from Prof. Levine regarding the scientific role of theory and computation. I apologize in advance to many other people, teachers, colleagues, students, friends, and supporters, who have deeply influenced my career and life, but unfortunately could not be mentioned as I ran out of space. You all know who you are, many of you appear in the citation list below, and I am grateful for everything you did for and with me. Having said that, none of the above could have happened without the support of my wonderful parents, Dr. Emila Freibrun and Prof. Israel (Izzy) Hod, who implanted in me curiosity and the love for science and supported me in any possible way; my amazing wife, Adi, who sacrificed so much so I could proceed with my career and supported me (and continues to do so) unconditionally throughout this long and fascinating journey; my perfect daughters Ophir, Ariel, and Elah for shining their light and teaching us the meaning of life; and my brothers and sister, Nir, Shahar, and Sivan, for serving as role models, each in their own field. Finally, it is far from being time for summaries. There are still many more little treasures to explore in my "ideas" email folder. The eternal dance between theory, computation, and experiment, in which I am honored to play even the tiniest role, continues.

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The 87th Annual Meeting of the Israel Chemical Society: April 3, 2024, Smolarz Auditorium, Tel Aviv University

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Introduction

The Annual Meeting of the Israel Chemical Society (ICS) has a long history since 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 occur in mid-February, the inter-semester break for all Israeli universities. Unfortunately, the Meeting of 2021 fell victim to the global COVID-19 pandemic, forcing a gap of 2.5 years between the 85th Meeting of February 2020 at the International Conference Center, Jerusalem, and the 86th Meeting of September 2022 at the David Intercontinental Hotel, Tel Aviv. That disruption of our usual schedule and the consequences of the war in the Gaza Strip forced us to postpone the 87th meeting several times. Finally, the ICS Executive Board decided to hold the meeting on April 3, 2024, and reduce it to a single day rather than the traditional structure of two days.

The chosen venue was the Smolarz Auditorium, located on the southern section of the Tel Aviv University campus. The building, completed in 2003, offers 5,000 square meters for diverse activities. Its layout blends the two different urban grids that regulate the campus. The fusion between the two main volumes of the building, the foyer and auditorium, creates outstanding views, and the main hall, with its 1,200 convenient seats, could accommodate the planned meeting perfectly.

Following ICS tradition, the chemistry departments of the six major research universities share responsibility for organizing these meetings in a six-year cycle in a constant 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. Thus, looking back at the ICS history of the past two decades, the Technion, for example, has taken responsibility for organizing the 68th Meeting (2003), the 74th Meeting (2009), the 80th Meeting (2015), and the 86th Meeting (2022). This year, following a previous decision of the ICS Executive Board, Ariel University joined this cycle for the first time. Thus, the organizing Committee included four members from the Department of Chemical Sciences, Ariel University: co-chairman Prof. Flavio Grynszpan, co-chairman Prof. Alex Schechter, Prof. Alex M. Szpilman, and Dr. Tomer Zidki, augmented by Prof. Norman Metanis of the Hebrew University of Jerusalem, and Prof. Micha Fridman of Tel Aviv University.

Another unique tradition the ICS has followed for over 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, thus enhancing their prospects of networking and scientific collaboration. Unfortunately, the large delegation of 10 scientists and 20 graduate students from Denmark prefered to visit Israel when the war ends. The ICS Board decided to postpone their participation to a later year.

Nevertheless, with its ambitious program, the one-day event provided an excellent opportunity to gather together many students, postdoctoral fellows, and scientists from around Israel, 18 months after the 86th ICS meeting, even without a foreign delegation. Over 500 participants enjoyed a diverse scientific program that included 16 plenary and keynote lectures in the main hall and two technical lectures in another. The 230 posters, all displayed at a single poster session, required an extension of the foyer by an external tent. The organizing committee selected four posters for the Best Poster Prizes awarded at the Prize Ceremony, which was held in the evening.

In addition to the scientific program, the ICS held its traditional General Assembly in the early afternoon, 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. A Gender Equality Power Hour occurred during the poster session, chaired by Mindy Levine of Ariel University. The prize ceremony, which took place in the evening, was preceded by a reception and light dinner for all participants.

The event attracted many sponsors, including the Weizmann Institute of Science, Tel Aviv University, Ben-Gurion University of the Negev, the Hebrew University of Jerusalem, Ariel University, the Technion, Bargal Analytical Instruments Ltd., Eldan Neopharm Group, and Tzamal D-Chem Laboratories.

The meeting featured a comprehensive commercial exhibition, with 13 providers showcasing a wide array of lab equipment, scientific instrumentation, chemicals, materials, analytical chemistry services, and publishing houses. The exhibitors included Arad-Ophir Information Specialists Ltd., Bargal Analytical Instruments Ltd., BioAnalytics Ltd., Bruker Scientific Israel Ltd., Labotal Scientific Equipment Ltd., LabSuit Projects Ltd., Rhenium Ltd., Tzamal D-Chem Laboratories Ltd., Gadot-Mercury, Eldan Neopharm Group, Medi-Fischer Engineering & Science Ltd., Merck, and Prime Lab Scientific Instruments Ltd.

The mix of excellent lectures, colorful poster sessions, exhibitions, and other activities created a vivid atmosphere with vibrant discussions, exchange of information, and social gathering, as reflected by the collage of photographs (Figure 1).

Opening Ceremony

Prof. Alex Schechter, co-chairperson of the organizing committee, opened the meeting and greeted the guests and participants: "Good morning, everyone. On behalf of the other co-chairperson, Prof. Flavio Grynszpan, and the organizing committee, I am delighted to welcome you to the 87th meeting of the Israel Chemical Society in Tel Aviv. It has been a while since the previous meeting. Before fully recovering from the Covid pandemic, the war and resultant upheavals forced us to organize this annual meeting in a reduced format. Furthermore, the international delegation from Denmark postponed their arrival to quieter times.

"Nevertheless, our resilient academic community has shown remarkable strength in dealing with the changing conditions. We have found innovative ways to continue our scientific work, teaching, and meeting in workshops and conferences. Despite the difficulties, it is crucially important that we continue our longstanding tradition of ICS meetings. This celebration of Israeli chemistry is a unique opportunity to share our enthusiasm for science and to recognize excellence in research, teaching, and other aspects of academic life. I wish you all an enjoyable meeting."

Prof. Ehud Keinan, president of the ICS, greeted the audience: "Good morning, everybody, and welcome to the 87th Meeting of the ICS. David Ben-Gurion once said that in Israel, 'Anyone who doesn't believe in miracles is not a realist.' Indeed, seeing over 500 participants, 230 posters, and an extensive exhibition in these challenging times is no less than a miracle, certainly when most other scientific conferences in Israel were canceled, postponed to some unknown date, or transferred to another location abroad. Many members of our community are experiencing losses, grief, and stress, and many are still on active duty in the army. At the same time, the length and quality of the academic year still need to be determined. The ICS Board's decision to take the risk and hold this meeting under the changing reality is a typical case of Israeli hutzpah. Condensing a two-day symposium into one day is non-trivial, and doing it for the first time without an organizing company is another miracle.

These achievements could only have happened with the coordinated effort and enthusiasm of many eager young people to meet friends and colleagues. I want to acknowledge them and all members of the organizing committee, most of them from Ariel University. It's the first time Ariel University has joined the cycle, so now it includes seven universities. Next year, it will be the turn of Bar-Ilan University to organize the 88th ICS Meeting in February 2025, and we hope the environment will allow for the participation of an international delegation.

I want to acknowledge the main sponsors of this meeting, including all chemistry departments at the Israeli research universities and Bargal, Eldan, and Tzamal companies. I thank Rinat Avital and Lee Reider, who manage the Smolarz Auditorium, and Benny Bashan, who organized the commercial exhibition. I thank the exhibitors, lecturers, and poster presenters, and I encourage all of you to visit the posters and the exhibition. Above all, I would like to thank my right-hand, Ms. Tali Lidor, the administrative manager of the ICS, who served as the organizing company. Without her, this event would not be possible. Tali has done most of the work, and I joined her team. I want to thank the ICS Executive Board, with whom we have worked for many years.

The Israel Chemical Society is older than the State of Israel, and we now celebrate the 90th birthday of the ICS. The Establishment of the ICS and its history is a fascinating story that started in 1933, when a group of chemists, mainly chemistry professors who fled Nazi Germany, gathered in Tel Aviv and formed the Association of Chemists in Palestine, which later changed its name to the ICS. I'm proud to serve more than 15 years as ICS president. This year is particularly challenging for me as I started my role as the IUPAC president.

Later tonight, we'll gather in this auditorium for an exciting evening, recognizing the achievements of 38 ICS Prize winners of the 2022 and 2023 cycles. Soon after the meeting, I'll issue a call to nominate candidates for all 2024 ICS prizes, and I

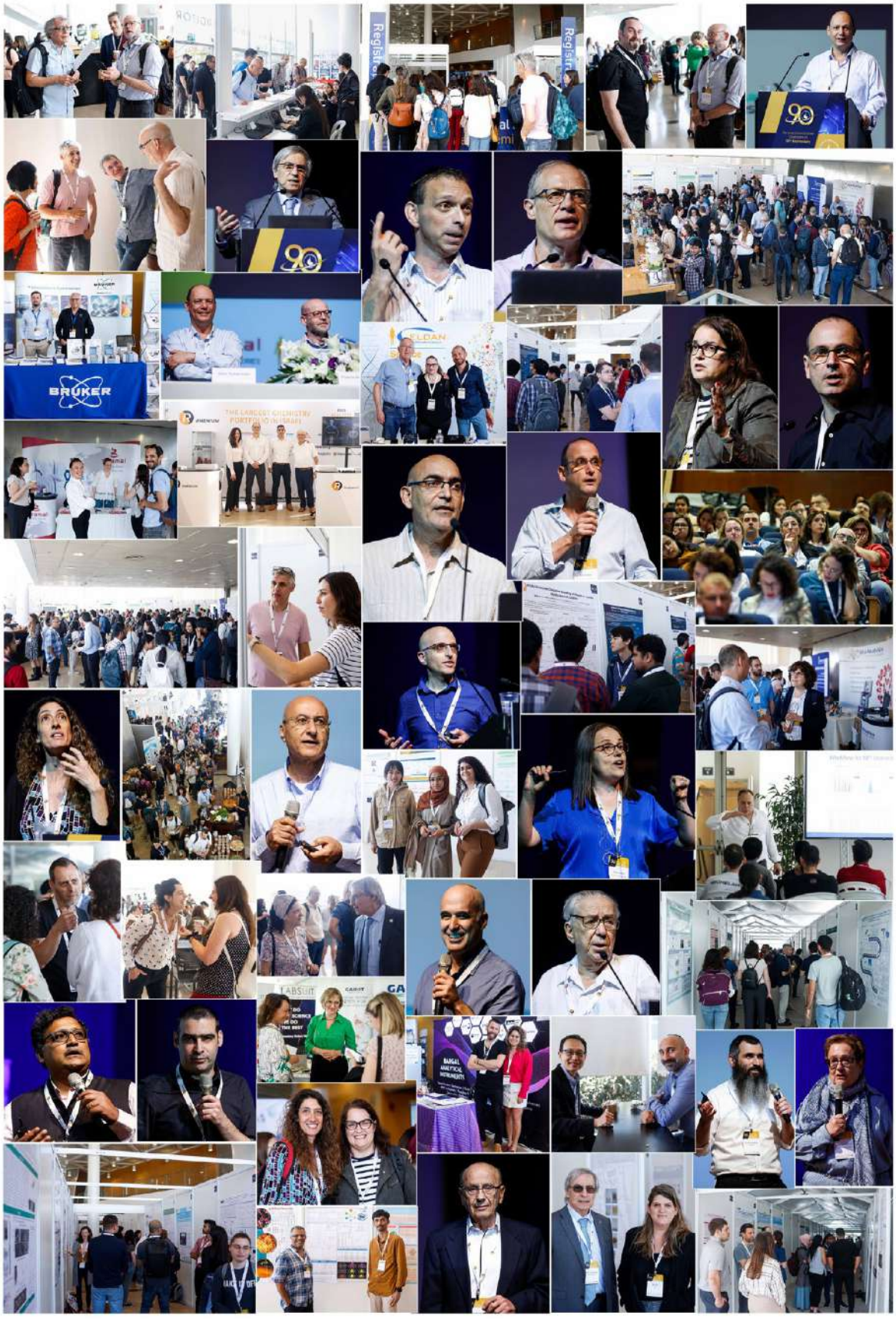

Figure 1. A collage of photos reflecting the general atmosphere throughout the 87th ICS meeting, including the lectures, posters, and commercial exhibition. Photos by Dror Sithakol.

will take this opportunity to focus on the gender issue. I am happy with the trend of steadily increasing gender equality in academia, although the list of ICS Prize laureates still needs to reflect this trend entirely. Although we cannot and should not influence the decision-making process of the specific prize juries, where gender equality exists, we must ensure that every gifted female scientist is nominated. And this responsibility goes to everybody because every registered ICS member can nominate other members as candidates.

Thanks again for participating in the 87th ICS Meeting; I wish you an enjoyable, highly fruitful experience!"

Lectures

Unlike the traditional two-day ICS meeting programs, which included 4-5 parallel sessions, the one-day format, and the venue's structure led the organizing committee to build a program of 16 lectures in the main auditorium, two technical lectures in a separate hall, and 230 posters.

Lucio Frydman of the Weizmann Institute of Science, 2022 ICS Prize of Excellence winner, lectured on "Nuclear Magnetic Resonance or Magnetic Resonance Imaging? Let's take both."

Oded Hod of Tel Aviv University, 2022 ICS-Tenne Prize winner, spoke about "Layered Ferroelectricity: from Geometric Measures to First-Principles Calculations."

Leeor Kronik of the Weizmann Institute of Science spoke about "Understanding optical properties of biogenic and bio-inspired molecular crystals: a first-principles perspective."

Sharon Ruthstein of Bar-Ilan University lectured on "The correlation between the gating mechanism of the human copper transporter, Ctr1, and the development of innovative biomarkers."

Eylon Yavin of the School of Pharmacy, The Hebrew University of Jerusalem, spoke about "FIT-PNAs as RNA sensors for Ovarian cancer diagnostics."

Doron Pappo of Ben-Gurion University of the Negev, 2023 ICS-Adama Prize winner, spoke about "Redox-Active 3rd-Transition Metal Catalysts for Dehydrogenative C–H Bond Coupling."

Raya Sorkin of Tel Aviv University spoke about "Membrane tension and membrane (hemi)fusion."

Shlomo Magdassi of The Hebrew University of Jerusalem, 2022 ICS Prize of Excellence winner, spoke about "From Gutenberg Bible to 4D printing."

Galia Maayan of the Technion lectured on "Bio-inspired electrocatalytic water oxidation."

Dan Meyerstein of Ariel University and Ben-Gurion University spoke about "The Mechanisms of the Fenton and Fenton-Like Reactions."

Malachi Noked of Bar Ilan University, 2023 ICS Young Scientist Prize winner, spoke about "Mitigating Electrode Material Degradation through Advanced Surface Modification Technique."

David Eisenberg of the Technion spoke about "Porous Materials: The Next Frontier in Energy Research."

Emanuel Peled of Tel Aviv University spoke about "Lithium and sodium metal batteries."

Idan Hod of Ben-Gurion University of the Negev, 2022 ICS Young Scientist Prize winner, spoke about "Molecular Manipulation of Heterogeneous Electrocatalysis Using Metal-Organic Frameworks."

Abhishek Dey of the Indian Association for the Cultivation of Science, West Bengal, India, spoke about "Factors Deciding the Selectivity of O_2, NO, CO_2, and SO_2 Reduction."

The 2024 ICS Prize Ceremony

An extended audience gathered in the main auditorium for an exciting evening, where an unprecedented number of 38 prize winners of the 2022 and 2023 cycles were recognized for their achievements (Figure 2). A festive reception, which marked a delightful transition from the intense scientific lectures to the prize ceremony, allowed for a significant population change. The arrival of many family members of the prize winners, including young children and elderly grandparents, resulted in an atmosphere that transformed gradually from a solemn science-focused program to a more joyful social event (Figure 3). The 1.5-hour ceremony took place at the main auditorium in the presence of a heterogeneous audience.

The 2022 ICS Prizes

The **2022 ICS Gold Medal** was awarded to **Prof. Ron Naaman** of the Department of Chemical Physics at the Weizmann Institute of Science for discovering the Chiral Induced Spin Selectivity (CISS) effect and explaining why nature preserved chirality persistently through evolution; and **Prof. Zeev Gross** of the Schulich Faculty of Chemistry, Technion, for pioneering the corrole chemistry, and impacting bio-inorganic chemistry, metal-based drug candidates and catalysis.

Prof. James Y. Becker of the Ben-Gurion University of the Negev became the **2022 Honorable Member of the ICS**

Figure 2. The ICS traditional poster displays all 38 prize winners who received their awards at the April 3rd ceremony.

Figure 3. A collage of photos reflecting the general atmosphere in the evening reception preceding the ICS Prize Ceremony. Photos by Dror Sithakol.

for his extensive contributions to organic electro-synthesis and electro-catalysis and for outstanding contribution to chemistry education at all levels.

The **2022 ICS Prize of Excellence** was awarded to **Prof. Shlomo Magdassi** of The Hebrew University of Jerusalem for developing micro and nanomaterials and their applications in delivery systems and functional printing; and **Prof. Lucio Frydman** of the Weizmann Institute of Science for his long-standing, seminal contributions to Magnetic Resonance.

The **2022 ICS Excellent Young Scientist Prize** was awarded to **Prof. Ori Gidron** of The Hebrew University of Jerusalem for his contribution to the fields of non-planar aromatic materials and macrocyclic chemistry and **Prof. Idan Hod** of Ben-Gurion University of the Negev for designing MOF-based platforms that manipulate heterogeneous electrocatalysis at the molecular level through secondary-sphere interactions.

The **2022 ICS-Dalia Cheshnovsky Prize for Excellence in Chemistry Teaching** was awarded to **Ms. Dafna Yam** of the Ohel-Shem High School, the Herzlia High School of Engineering in Tel Aviv, and the Ort High School for the Arts and Sciences, Ramla, for teaching chemistry with professionalism, dedication and creativity, and guiding chemistry teachers, while assimilating new teaching methods

and innovative pedagogy, giving attention to every student, at all times, with great patience and pleasant manners.

The **2022 ICS-Uri Golik Prize for an Excellent Graduate Student** was awarded to **Dr. Efrat Resnick** of the Weizmann Institute of Science for developing chemical probes for protein targets and a specific inhibitor against SARS-CoV-2 protease.

The **2022 ICS-Shahar Prize for the Excellent Administrative Assistant** was awarded to **Ms. Liat Presman**, Academic staff and Dean's office coordinator at the Schulich Faculty of Chemistry, Technion. She received the prize for her remarkable professional and creative management with passion and dedication, work ethic, human relations, and outstanding organizational skills manifested by voluntarily expanding her contributions beyond the formally expected.

The **2022 Tenne Family Prize in memory of Lea Tenne for Nanoscale Sciences** was awarded to **Prof. Oded Hod** of the School of Chemistry at Tel Aviv University for predicting structural superlubricity in heterogeneous layered material contacts and developing simulation tools and geometric measures for nanoscale 2D materials.

The **2022 ICS-Adama Prize for Technological Innovation** was awarded to **Prof. Aharon Blank** of the Schulich Faculty of Chemistry, the Technion, for developing new methodologies in magnetic resonance and applying them to science, technology, and medicine.

Figure 4. Award ceremony of the 2022 ICS Prizes. First row from left: Excellent Graduate Students with their university representatives: David Azulay (with Shlomo Magdassi of The Hebrew University of Jerusalem), David Zitoun of Bar-Ilan University receives the award for Ariel Friedman, Itai Massad (with Aharon Blank of the Technion), Noy Nechmad (with Gabriel Lemcoff of Ben-Gurion University), Moshe Kol of Tel-Aviv University receives the award for Inbal Oz. Second row: Golokesh Santra (with Lucio Frydman of the Weizmann Institute of Science) and Alina Sermiagin (with Alex Szpilman of Ariel University). Lucio Frydman receives the ICS-Uri Golik award for Efrat Resnick of the Weizmann Institute (with Uri Golik, Eran Golik, and Moshe Cohen), Oded Hod receives the ICS-Tenne award (with Reshef Tenne), Resgef Tenne receives the ICS recognition for his extended support of the ICS). Third row: Aharon Blank receives the ICS-Adama Prize (with Efrat Lifshitz and Itsik Bar-Nahum of Adama), Liat Presman receives the ICS-Shahar Prize (with Efrat Lifshitz and Dani Shahar), Dafna Yam receives the ICS-Dalia Cheshnovsky Prize for Excellence in Chemistry Teaching (with Dorit Teitelbaum, Ori Cheshnovsky, and Dani Shahar), James Y. Becker becomes a Honorable Member of the ICS (with Gabriel Lemcoff), Ori Gidron receives ICS Excellent Young Scientist Prize. Fourth row: Ori Gidron receives the ICS Excellent Young Scientist Prize (with Gabriel Lemcoff), Lucio Frydman receives the ICS Prize of Excellence, Shlomo Magdassi receives the ICS Prize of Excellence, Ron Naaman receives the ICS Gold Medal, Zeev Gross receives the ICS Gold Medal. Photos by Dror Sithakol.

The 2022 ICS Prize for an Excellent Graduate Student was awarded to seven graduate students: **David Azulay** (The Hebrew University of Jerusalem), **Ariel Friedman** (Bar-Ilan University), **Itai Massad** (Technion), **Noy Nechmad** (Ben-Gurion University), **Inbal Oz** (Tel-Aviv University), **Golokesh Santra** (Weizmann Institute of Science), and **Alina Sermiagin** (Ariel University).

The 2023 ICS Prizes

Prof. Matityahu (Mati) Fridkin of the Weizmann Institute of Science and **Prof. Chaim Gilon** of the Hebrew University of Jerusalem became **Honorable Members of the ICS** for their seminal contributions to the science of peptides and proteins from synthesis to therapeutic agents and for training many followers in academia and industry.

The **2023 ICS Excellent Young Scientist Prize** was awarded to **Prof. Malachi Noked** of Bar-Ilan University for his pioneering contributions to solid-state batteries, high-energy-density batteries, electromobility, thin functional films, and innovative materials; and **Prof. Nadav Amdursky** of the Schulich Faculty of Chemistry, the Technion, for developing new ways of studying and utilizing proton transfer reactions in biological materials, biopolymers, and dynamic systems.

The **2023 ICS-Dalia Cheshnovsky Prize for Excellence in Chemistry Teaching** was awarded to **Ms. Rachel Kelner** of the Amit Yeshurun Ulpanit, Petah Tikva, for four decades of excellence in chemistry teaching, for developing innovative teaching methods, educating students and teachers in different channels, and for evaluating and analyzing the matriculation exams in chemistry.

The **2023 ICS-Uri Golik Prize winner for an Excellent Graduate Student** was awarded to **Mr. Bar Cohn** of the Schulich Faculty of Chemistry, the Technion, for his outstanding contributions to ultrafast dynamics of the interaction between molecular vibrations and optical cavities at ambient conditions.

The winner of the **2023 ICS-Shahar Prize for Excellent Administrative Assistant** was awarded to **Ms. Elena Borodina**, administrative manager of the Department of Chemical Sciences at Ariel University, for her remarkable professional and creative management with passion and dedication, work ethic, human relations, and outstanding organizational skills.

The **2023 Tenne Family Prize for a young scientist in memory of Lea Tenne for Nanoscale Sciences** was awarded to **Dr. Benjamin Palmer** of the Department of Chemistry of Ben Gurion University for his outstanding work on the characterization of unique biogenic nanostructures and the understanding of their structure-function relations in living organisms.

The **2023 ICS-Adama Prize for Technological Innovation** was awarded to **Prof. Doron Pappo** of the Ben-Gurion University of the Negev for developing innovative oxidative coupling methods based on abundant transition metal catalysts for practical synthesis of complex molecules.

The **2023 ICS Prize for an Excellent Graduate Student** was awarded to seven graduate students: **Itamar Liberman** (Ben-Gurion University), **Poulami Mukherjee** (Ariel University), **Ilan Shumilin** (The Hebrew University), **Benjamin Sorkin** (Tel-Aviv University), **Tamar Wolf** (Weizmann Institute of Science), **Anna Yucknovsky** (Technion), and **Shani Zev** (Bar-Ilan University).

The **2023 ICS award for the green chemical industry** was awarded to All Recycling and its CEO, **Gadi Reichman**, for applying advanced technology to recycle electronic waste and produce valuable raw materials, thus reducing the need to mine limited natural resources and lowering energy costs.

The **2023 ICS-Peled Prize for a high school graduate for an Excellent Chemistry Project** was awarded to **Yonatan Shapira** and **Ethan Amiran** of the Jerusalem's Israel Arts and Sciences Academy. Yonatan Shapira received the Prize for his research project "Production of atomic chips" under the supervision of Prof. Liraz Chai and Dr. David Azulay of the Institute of Chemistry, The Hebrew University of Jerusalem. Ethan Amiran received the Prize for his research project, "light-emitting perovskite nanoparticles after replacing halides and cations," supervised by Prof. Lioz Etgar and Mrs. Tal Binyamin of the Institute of Chemistry, The Hebrew University of Jerusalem.

Prof. Reshef Tenne was awarded recognition for his long-standing support of the ICS through the Tenne-family prize. Tenne responded, "I wish to congratulate the recipients, Prof. Oded Hod of Tel Aviv University and Dr. Ben Palmer of Ben-Gurion University, of the Tenne Family Prize in memory of Lea Tenne Z"L. Together with my family, we thank the Israel Chemical Society for hosting this prize. We are privileged to have such a list of excellent scientists to be chosen year after year (for the last 12 years) to receive this important recognition. This is the best way for me and my family to commemorate the legacy of my late first wife, Lea, who was not a scientist but was very attached to science. This prize is intended to recognize the contributions of Israeli scientists in this dynamic field of research, thereby promoting excellence in science in the country.

Figure 5. Award ceremony of the 2023 ICS Prizes. First row from left: Excellent Graduate Students with their university representatives: Itamar Liberman (with Idan Hod of Ben-Gurion University), Alex Szpilman receives the award for Poulami Mukherjee of Ariel University, Ilan Shumilin (with Shlomo Magdassi of The Hebrew University), Benjamin Sorkin (with Moshe Kol of Tel-Aviv University), Tamar Wolf (with Lucio Frydman of the Weizmann Institute), Second row: Anna Yucknovsky (with Efrat Lifshitz of the Technion), and Shani Zev (with Dan Major of Bar-Ilan University), Bar Cohn receives the ICS-Uri Golik award (with Uri Golik, Efrat Lifshitz, Eran Golik and Moshe Cohen), Benjamin Palmer receives the ICS-Tenne award (with Reshef Tenne), Doron Pappo receives the ICS-Adama Prize (with Itsik Bar-Nahum of Adama), Third row: Elena Borodina receives the ICS-Shahar Prize (with Dani Shahar), Rachel Kelner receives the ICS-Dalia Cheshnovsky Prize for Excellence in Chemistry Teaching (with Dorit Teitelbaum, Ori Cheshnovsky, Dani Shahar, and Dafna Yam), Yonatan Shapira (left) and Ethan Amiran (right) receive the ICS-Peled Prize for a high school graduate for an Excellent Chemistry Project (with Dorit Teitelbaum, Nehama Peled, and Michael Peled), Nehama and Michael Peled receive the ICS recognition for their extended support of the ICS, Gadi Reichman of All Recycling receives the ICS award for the green chemical industry. Fourth row: Chaim Gilon becomes an Honorable Member of the ICS, Matityahu Fridkin becomes an Honorable Member of the ICS, Matityahu Fridkin, Emma Fridkin, Noemi Gilon, and Chaim Gilon, Malachi Noked receives the ICS Excellent Young Scientist Prize (with David Zitoun), Efrat Lifshitz of the Technion receives the ICS Excellent Young Scientist Prize for Nadav Amdursky. Photos by Dror Sithakol.

POSTER PRIZES

The organizing committee selected four posters for the Best Poster Prizes awarded at the evening Prize Ceremony.

Poster ICN-18 "Enhancing Stability and Solar Cell Efficiency of $CsPbBr_3$ Nanowire Arrays Grown on Anodized Aluminum Oxide: Insights into Light-Matter Interactions," by **Neena Prasad** and Lena Yadgarov of the Department of Chemical Engineering, Ariel University.

Poster OOC-05, "Stereoselective synthesis of 1,n dicarbonyl compounds through palladium catalyzed ring opening/isomerization of densely substituted cyclopropanols," by **Charlotte S. Teschers**, Anthony Cohen, and Ilan Marek of the Schulich Faculty of Chemistry and the Resnick Sustainability Center for Catalysis, Technion.

Poster PC-15, "Investigating Radical Chemistry With Synchrotron Radiation," by **Nadav Genossar-Dan** and Joshua H. Baraban of the Department of Chemistry, Ben Gurion University.

Poster EC-19, "Nitrate Reduction to Ammonia: Assessing the Electrocatalytic Behavior of Cu_3N," by **Paz Stein**, Ronen Bar-Ziv, and Maya Bar-Sadan of the Department of Chemistry, Ben Gurion University, and Department of Chemistry, Nuclear Research Center Negev.
The full report was published in the Israel Journal of Chemistry.

The Israel Chemical Society
(ICS: www.chemistry.org.il)