Institute Spotlight

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The Lise Meitner-Minerva Center for Computational Quantum Chemistry: 18 Years of Israeli-German Collaboration

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Abstract: We tell the story of the Lise Meitner-Minerva Center, its establishment and activities, its members and their scientific activity, and its instrumental role in weaving intense relationships with the theoretical community in Germany, and in amalgamating the Israeli community of computational quantum chemistry into a national center that enjoys a high international reputation.

1. Introduction

The idea to create a computational quantum chemistry (CQC) center in Israel was motivated by the perception that in the 21st century, CQC will become chemistry's 3rd power, alongside experiment and theory. In 1966, Mulliken stated that "… the era of computing chemists, when hundreds if not thousands of chemists will go to the computing machine instead of the laboratory for increasingly many facets of chemical information, is already at hand." It took only two decades to witness Mulliken's vision coming true, and computational quantum chemistry becoming a fundamental tool that is a "must-have" tool in chemical research rather than a "nice-to-have" tool!

2. Establishing the Lise Meitner-Minerva Center for Computational Quantum Chemistry

In 1994, there were only a few research groups that practiced CQC in Israel. Among them were those of Yitzhak Apeloig at the Technion (TEC) and of Sason Shaik at the Hebrew University (HU), who had been discussing what could be done to change this situation and meet the demands of the 21st century. At that time, the school of CQC in Germany was one of the world's leaders. On this background, Shaik and Apeloig (S&A) decided to establish a center *wherein computations, theory and experiment interact and enrich thereby each other*. Interaction with German theoreticians was already ongoing, and hence, it was thought that these connections could become the driving force for the internationalization of such a center. And this is how the story unfolded.

The original vision was to form a center of excellence and competence that would eventually possess a critical mass of highly qualified researchers, and in which the powerful tools of modern computational quantum chemistry and quantum chemical thought would be applied to central themes covering the gamut of chemistry: from fundamental concepts, such as the transition state and aromaticity, to questions of structure and reactivity, all the way to more practical problems, such as the chemistry of novel materials, catalysis by transition metals and enzymes, and more. The center was to also serve as a focal institution for training and educating a generation of qualified young investigators, doctoral students, and postdoctoral fellows. As both groups had had productive collaborations with German research groups, S&A decided to submit a proposal to the Minerva Foundation, which had been supporting such know-how centers in Israel since 1979. Under this umbrella, another very important goal of the center was to foster collaboration and synergy with the German CQC school and strengthen German-Israeli scientific ties. As both S&A had been collaborating with experimentalists throughout their careers, and as one of them (Apeloig) was engaged in dual research combining experiment and computations, they thought that a major theme of such a center should be *the interplay of theory and experiment*.

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The Minerva Foundation requires all its prospective centers to prove solid collaboration and support from leading scientific groups in Germany. Both S&A spent quite a few trips back and forth between Germany and Israel (including longer sabbatical periods) to strengthen existing ties (e.g., with H. Schwarz, L. S. Cederbaum and P. v. R. Schleyer) and create new ones (e.g., with S. D. Peyerimhoff and J. Sauer). This last aspect makes an interesting story by itself, which may be told on another occasion. In the end, we were fortunate to have the support of five top German scientists: L. S. Cederbaum, S. D. Peyerimhoff, J. Sauer, P. v. R. Schleyer, and H. Schwarz. With this important support, S&A drafted the first version of the proposal. After several rounds of rewriting, in which Helmut Schwarz and Sigrid Peyerimhoff provided important input, and Ms. Charlotte Goldfarb, from the Research and Development Authority (RDA) at HU, provided decisive advice,[1] the Minerva proposal to establish a CQC center jointly at the Hebrew University and the Technion, was submitted on December 23rd, 1993.

S&A were fully aware that the competition would be fierce, since only 2–3 proposals were to be approved out of approximately 30 proposals that were submitted by all universities. It was also known that due to budgetary constraints at the Minerva Foundation, the approval of any new Minerva center was due to transpire only one to two more years after the submission. In view of these initial small odds, we were delighted when the center was approved in 1995! Subsequently, an advisory board was selected and it constituted of three German scientists (Helmut Schwarz, Sigrid D. Peyerimhoff, and Joachim Sauer) and three Israeli scientists (Nimrod Moiseyev, Eli Grushka, and Addy Pross). Minerva nominated Prof. Helmut Schwarz as the chairman of the *Beirat*, which is the German term for an Advisory Board. In those moments, it dawned on us that computational quantum chemistry in Israel had entered a new era.

The Center was inaugurated on July 7th, 1997, with a scientific symposium (see in Figure 1 the get together on the eve of the inauguration day at Shaik's apartment in Jerusalem). Sason Shaik was nominated as the director and Yitzhak Apeloig as the codirector. This past July 2015, the Lise Meitner Center celebrated 18 years of productive scientific achievements and successful collaborations with German scientists, theoreticians and experimentalists, and with the worldwide community of computational and theoretical chemists. In the course of these 18 years, the Lise Meitner Center has become an entity of high international repute.

2.1 Selection of a Name for the New Center

Naming Minerva Centers is also a story that deserves a separate telling. Traditionally, Minerva centers in Israel have been named after Jewish scientists who were persecuted during the reign of the Nazi regime.[2] After a discussion during the 1996 WATOC Meeting in Jerusalem, on names like Schrödinger and Born, who were founding fathers of quantum mechanics, some difficulties became apparent. Schrödinger's impeccable history during the rise of the Nazi regime was later tarnished when Austria came under this regime. The naming of the center after Born was also not unanimously accepted, despite the Jewish roots of Born. Following this discussion, S&A decided to call the Center after a prominent woman scientist (our wives were in fact the driving force for that), not necessarily a quantum mechanics pinoeer. Thus, the Center was named after Lise Meitner,[3] an Austrian-German Jewish physicist (Figure 2) who worked in close collaboration with Otto Hahn in Berlin between 1912 and 1939, and became one of the major figures in the emerg-

Figure 1. The party on the eve of the inauguration day of the Lise Meitner Center. Standing from right to left on the second row are: Shabtai Dover (RDA@HU), Yitzhak Apeloig, Mr. Dietmar Nickel (Minerva), and the members of the first *Beirat*, Sigrid D. Peyerimhoff, Helmut Schwarz, Nimrod Moiseyev, Addy Pross, and Eli Grushka. Standing in the front row is Sason Shaik.

Figure 2. Lise Meitner in her youth.

ing field of radioactivity; a codiscoverer of a new element, Protactinium; one of the pioneers in the establishment of the structural model of the nucleus, and the first (together with her nephew, Otto Robert Frisch, also a Jewish scientist persecuted by the Nazi regime) to understand and theorize the concept of nuclear fission, to predict its outcome in a manner amenable to experimental proof, and to predict the existence of a chain nuclear reaction. Although Meitner converted to Catholicism at an early stage of her life, the tragic fate of the Jews in Europe pursued her, and in 1938, after Austria's "*Anschluss*," she was forced to abandon her academic position in Berlin and flee to Sweden, where she was offered a position in the Manne Siegbahn Institute. In the Manne Siegbahn Institute, Lise Meitner found herself being scientifically isolated from her peers for the rest of World War II. Eventually, in 1944 the Nobel committee overlooked her major contribution and the Nobel Prize for "the discovery of the fission of heavy nuclei" went to Otto Hahn alone, which many think was a mistake of the Nobel committee. Interestingly, the Lise Meitner Center is one of the very few Minerva centers to be named after a women scientist, attesting to the very small number of women who were active in science in the 1930s. Thus, Lise Meitner was a pioneering scientist discriminated for having two ″faults″: being both Jewish and a woman! We have chosen well… Naming our Center after her was a very good idea.

3. From a Two-site Center to a National Center

The Lise Meitner Center (LMC) started as a bi-institutional center at the Technion (TEC) in Haifa and the Hebrew Universiy (HU) in Jerusalem. It involved groups who did research both in theory and in experiment. Except for the two founders (S&A), the members were: David Avnir, Chava Lifshitz, Mordecai Rabinovitz, and Zvi Rappoport (from HU); and Menachem Kaftory, Ehud Keinan, Asher Mandelbaum, Uri Peskin, and Amnon Stanger (from TEC). Subsequently, Shlomo Yitzchaik and Roi Baer, who were both new recruits at the HU, joined the Center (since then Roi Baer moved to the Fritz Haber Center while Shlomo Yitzchaik shifted to Farkas Center).

However, S&A soon realized that to have a critical mass, it is necessary to create a multi-institutional center. And as time went by, groups of newly recruited young faculty members from the Weizmann Institute of Science (WIS), then from Bar-Ilan University (BIU), Tel Aviv University (TAU), and Ben Gurion University (BGU) were invited to join the Center. These groups were joined by new recruits from the two founding institutes, such that, from the mid-2000s, the Center has been expanded to include the research groups of David Avnir, Avital Shurki, Mordecai Rabinovitz, Zvi Rappoport, Sason Shaik, Roy Shenhar, and Roie Yerushalmi (HU); Yitzhak Apeloig, Menachem Kaftory, Asher Mandelbaum, Ilan Marek, Uri Peskin, and Amnon Stanger (TEC); Gershom Jan Martin, the late Michael Bendikov, and Leeor Kronik (WIS); Dan Thomas Major (BIU); Oded Hod (TAU); and Sebastian Kozuch (BGU). Two of the members (Chava Lifshitz and Michael Bendikov) passed away after long years of battling cancer, and one of them, Michael Bendikov, at a tragically young age of 42 and at a time when his scientific career was sky-rocketing. Some of the members (Kaftory, Mandelbaum, Rabinovitz, Rappoport) retired, and some moved to other Minerva centers (Baer, and Yitzchaik) or stopped their activity in the LMC (Keinan). The final membership of the center stabilized at 14 research groups, including those of the two founders.

In retrospect, the multi-institutional nature of the LMC has created added visibility and diversity in the research topics. This has been accompanied by strong commitment that has transcended institutional boundaries. *The LMC has become a true national center, with the sense of the unity of a team*. Moreover, the establishment of LMC has also significantly broadened the ties with the CQC community in Germany and with the community of theoretical and computational chemists worldwide, as well as with several experimental groups in Israel and abroad.

4. Achievement of Excellence and International Repute

4.1 Goals of Excellence

The main goals of the LM Center since its inception, have been the following: a) to create a platform for excellence and intense science where theory and experiment work in synergy in a wide range of chemistry fields; b) to intensify the connections between Israeli scientists in CQC by creating a critical mass, and encouraging young PhD students (mainly from Israel) and postdocs to practice CQC; c) to weave long-term German-Israeli scientific relations; and d) to aim for high visibility and international repute. These goals have ultimately defined the Center's programs, which have led to the achievement of excellence and visibility.

Important elements in achieving these goals are leadership, excellence of the research groups and productive scientific programs, which give the Center purpose and the ability to communicate on an international scale. The leadership emerged from a very close collaboration between the *Beirat* and the directors. This leadership was also behind the approval and implementation of the Center's high-level and productive programs. Let us discuss first the role of the *Beirat*.

4.2 The Role of the *Beirat*

The *Beirat* plays a very important role in the operation of a Minerva center like the one we had in mind. An almost yearly *Beirat* meeting takes place, in which the director of the center reports on the scientific activities of the center during the past year or so, and makes suggestions (scientific and financial) which require approval. The director's presentation is followed by a discussion between the *Beirat* members and the two directors. The *Beirat* approves the budget of the center, advises and approves/disapproves the nominations of new members to the center, approves/disapproves new programs, modes of fund allocation, and decides who will be the director of the center. Without these discussions, which endow the center with a sense of purpose and continuity, no center will be successful. This is the strength of the Minerva program, which with a rather modest amount of money is able to establish active and purposeful research centers.

Several years after the inception of the LMC, a few of the original *Beirat* members (see Figure 1) stepped down (following the Minerva guidelines) and new members were appointed. The current *Beirat* members are W. Thiel and P. R. Schreiner from Germany, and A. Goldblum, D. Milstein, and Z. Gross from Israel (Figure 3). H. Schwarz has remained the chairman since the Center's inception to this day. Thus, in many respects, the LMC has enjoyed a continuity of leadership. This has been attended, in turn, by strong collaboration and commitment between the *Beirat* and the directors, which has brought about the implementation of productive programs. The Lise Meitner Center was fortunate to have throughout its years of existence a highly committed *Beirat* that has provided the Center with good advice and pushed the directors to excel, and has, thereby, played a major role in the rise of the LMC to prominence.

Figure 3. The *Beirat* Members of the LMC starting in the early 2000s. From left to right: H. Schwarz (Chairman), P. R. Schreiner, and W. Thiel (from Germany), A. Goldblum, D. Milstein, and Z. Gross (from Israel).

4.3 The Professional Staff

Very early on, S&A realized that the achievement of excellence and international reputation required durable maintenance and technical know-how in the Center. For this purpose, it was decided to employ and support two such individuals who were deemed capable of providing the requisite know-how. Dr. Miri Karni at TEC and Dr. David Danovich at HU have filled these positions ever since the nascence of LMC. As such, they have become indispensable pillars in keeping the Center at a high professional level by providing support and scientific advice to all the students and postdocs in the Center, as well as to other researchers in Israel who are interested in applying computational methods to their research.

4.4 The LMC Members, Their Research, and Achievements

A most important cornerstone in building excellence is the careful selection of its research groups (see names and research interests of the Center members below). In line with the main goal of the LMC, the groups chosen to join the Center involved theoreticians and experimental group leaders, who were outstanding in their research and also interested in applying computational methods to their research. The member groups carried out research in fields ranging over organic, organometallic and silicon chemistry, catalysis, bio-related research, nano-related studies, in developing fundamental concepts (e.g. chemical bonding, aromaticity), as well as computational method development. More details are given below.

4.4.1 Main Research Interests of the LMC members

The members are listed alphabetically below.

Yitzhak Apeloig: Theory and experiment in synergy for studying various aspects of organosilicon chemistry. In particular, multiple bonds to silicon, low-valent silicon compounds, reactive intermediates such as silylenes, silyl anions, cations and radicals, metal substituted silanes, etc, as well various mechanistic problems in organic and organometallic chemistry.

David Avnir: The group has originated the notion that structural chemistry is too rich to be described with the coarse binary language of either being or not being symmetric or chiral. As such, the group has developed the continuous symmetry and continuous chirality measures (CSM and CCM), which have been applied across chemistry and biochemistry, and have revealed correlations between observables and CSM/CCM. The mathematical tools are available at http://www.csm.huji.ac.il/new//.

Oded Hod: Theoretical studies of the mechanical, electronic, magnetic, and transport properties of systems at the nanoscale. On top of basic science questions, the design of technologically applicable nanoscale material properties for future applications in fields such as nanoelectronics, nanospintronics, accurate and sensitive chemical detection, and nano-mechanical devices, is being pursued. A combination of in house developed codes, along with commercial computational chemistry packages is used.

Sebastian Kozuch: Uses computational tools to dissect catalytic cycles in all their facets: mechanistic networks; kinetic analysis; quantum methodology; and bonding and reactivity patterns. This approach permits the comparison of experimental and computational catalytic studies, and even to predict new, more efficient catalysts.

Leeor Kronik: First principles quantum mechanical calculations which predict properties of new materials from only the atomic number and mass of the atomic species involved. Using the laws of quantum physics, in conjunction with density functional theory and many-body perturbation theory, enables the group to achieve understanding of novel electronic, optical, and magnetic properties of materials and interfaces, in terms of their microscopic properties.

Dan T. Major: Theoretical study of enzymatic and solution-phase reactions using state-of-the-art combined quantum mechanics/molecular mechanics Hamiltonians; theoretical study of lithium battery properties and photovoltaics.

Ilan Marek: The group's vision is to provide answers to challenging synthetic problems in a manner that couples efficiency and elegance; in particular, C–C bond-forming processes, which efficiently create multiple stereocenters in a single-pot operation. Theoretical calculations in tandem with experiment enable the achievement of efficient and general synthetic protocols by providing understanding of the origins of chemo- and stereo-selectivity.

Gershom (Jan) Martin: The group engages in: a) Method development: i) the "W4 theory" (Weizmann-4), which offers unprecedented accuracy at still-tractable computational cost; and ii) DFT development centered mostly on more "universal" functionals. The BMK functional was the first to yield similar accuracy for equilibrium thermochemistry and barrier heights, while the recent double hybrid B2GP-PLYP functional offers accuracy and universality similar to composite and costly ab initio methods. b) Application of DFT methods for studying catalysis by late transition metals, renewable energy, and hydrogen storage, all in collaboration with experimental groups.

Uri Peskin: The group studies electronics of single molecules and quantum dots, and develops theoretical approaches to meet the challenges of dynamics in open quantum systems out of equilibrium.

Sason Shaik: The group's topics of interest range from bonding in small molecules and new bonding motifs, through to organic reactivity, and all the way to enzymatic and bioinorganic reactivity in the field of hydrocarbon oxidation and functionalization.

Roy Shenhar: The group studies the influence of molecular-scale interactions on the morphology of polymers and nanocomposite films. Insights gained by these studies are used to aid chemical design in developing polymer-based self-assembly strategies.

Avital Shurki: The group studies the reactivity of small molecules as well as large biological systems, and in particular, enzymes. The calculations focus on valence bond approaches and utilize the special chemical insight these approaches provide to understand and develop ways to further improve reactivity.

Amnon Stanger: DFT and *ab initio* methods are used to study principal chemical properties in conjunction to experiments. A wide range of subjects are studied, one example is the study of the nature of aromaticity. NICS-based methods (NICS-scan, σ-only model and NICS-XY-scan) for quantitative assessment of dia- and para-tropicity (aromaticity and anti-aromaticity) have been developed and integrated into Aroma – a Python program which automated all these methods and it is available in http://Schulich.technion.ac.il/Amnon Stanger.htm.

Roie Yerushalmi: The group focuses on the synthesis of nanostructures and the understanding of unique reactivity characteristics related to the nanoscale. The research combines synthetic methods for the formation of nanostructures with controlled chemical composition and the large scale deployment and assembly of the nanostructures. CQC is applied to understand the nanostructure properties.

Figure 4 shows a collage of representative research projects of the LMC members.

4.4.2 Awards and Distinctions

The excellent research achievements of the members of the Center have been underscored by many prestigious national and international awards. These include: the Israel Prize; the Israel Chemical Society Excellence Award; the Kolthoff Award; the Alexander von Humboldt Award; the Schrödinger Medal; AAAS (American Association for the Advancement of Science) Fellows selection; honorary foreign membership of the American Academy of Arts and Sciences; membership of Academia Europea; membership of the International Academy of Quantum Molecular Science (IAQMS); selection to be included in *175 Faces in Chemistry*; the Sol-Gel Lifetime Award; the F. S. Kipping Award of the American Chemical Society; the Wacker Prize; Jenssen Pharmaceutica Prize; the Order of Merit of Germany; the August Wilhelm von Hofmann Medal of the German Chemical Society; The Dirac Medal; the France-Israel Academic

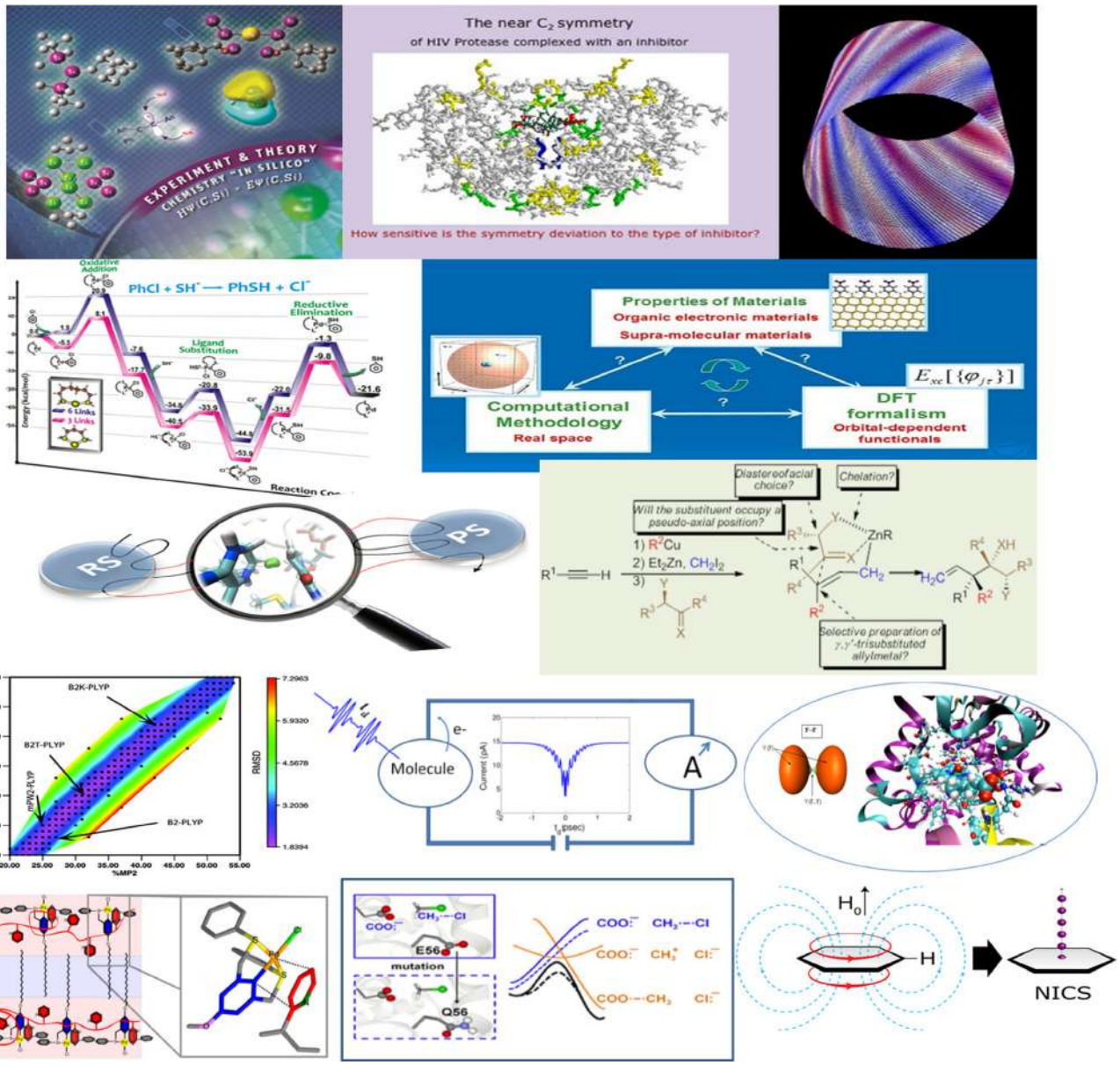

Figure 4. Representative research projects of the LMC members (arranged alphabetically): 1st row (from left to right): Y. Apeloig, experiment and theory of organosilicon chemistry and organic reactive intermediates; D. Avnir, symmetry and chirality; O. Hod, chiral registry patterns in double walled nanotubes; 2nd row: S. Kozuch, potential energy surface of a catalytic cycle;[4a] L. Kronik, main research interests; 3rd row: D. T. Major, enzymatic reaction; I. Marek, single pot creation of three new carbon-carbon bonds and two to three stereogenic centers, including an all-carbon quaternary stereocenter; 4th row: G. Martin, performance benchmark of DFT PLYP functionals developed by his group;[4b] U. Peskin, a molecular electronic junction;[4c] S. Shaik: from bonding in small molecules all the way to enzymatic and bioinorganic reactivity; R. Shenhar, Function-Structure relationship: Molecular Interactions Influencing Polymeric Structure;[4d] A. Shurki, nucleophilic substitution of a haloalkane in haloalkene dehalogenase (DhlA); A. Stanger, NICS(scan) method.

Award for Excellence; The Chaim Weizmann Research Award; The Journal of Physical Organic Chemistry (JPOC) award for "early excellence"; the DuPont Young Professor Award; the Krill Prize; and more. Some of the above prizes were won by several of the more established members, and others by the younger members. In addition, our younger members have won the prestigious ERC Advanced grant and ERC Starting grants, and/or have been elected members of the Israel Young Academy. It is also gratifying to note that many of the students and postdocs of the LMC went on to have their own academic careers in Israel and abroad. All these distinctions of the Center members and its researchers constitute a solid evidence for the excellence and high visibility of the Center.

Since its inauguration, the members of the Center have published more than 1000 papers bearing the LMC name,

in leading international scientific journals. Many of these include collaboration with German scientists. The members of the Center have raised many tens of millions of dollars in research money, sometimes in a ratio of almost 20:1 to the yearly interest from the Center's endowment, which served mostly to support the professional staff, provide some seed money and fellowships for new research, the yearly conference, administrative help, the purchase of computing equipment and its maintenance.

4.5 The Center's Programs

Several scientific programs, detailed below, were created by the Center to fulfill its goals of excellence and to strengthen the ties to German science. *These programs also created a sense of unity in the Center, like in a good orchestra.*

4.5.1 Scientific Symposia

The first program is a yearly international conference with the participation and lectures of outstanding computational chemists from abroad and of the Center's members. These symposia always include sizeable and lively poster sessions where students and postdocs of the Center have the opportunity to showcase their research and discuss it with their peers and senior scientists. Among the international lecturers in these conferences are award winners of the LMC, i.e., the Lise Meitner Lectureship (LML) Awardee and the Outstanding Young German (OYGA) Awardee (see below).

The Center's international conferences have usually coincided with the *Beirat* meetings, but occasionally these conferences take place in the founding institutions independent of the *Beirat* meetings. Details on the yearly conferences which have taken place during the past 18 years can be found in the website of the LMC;[5] below we describe a sample of these events.

1) The 1998 symposium, *Frontiers in Electronic Structure Calculations*, was held at the Technion with the following international speakers: K. Morokuma, M. S. Gordon, R. A. Freisner, F. Weinhold, S. D. Peyerimhoff, J. Sauer, J. Gauss, A. Dreuw, W. Koch, and H. Schwarz. All other speakers were members of the Center (like Shaik, Apeloig, Avnir, …) and other Israeli theoreticians (e.g., B. Gerber).

2) The 2000 symposium, *Electronic Structure: Interplay of Theory and Experiment and Perspectives of Research Activities*, was held at HU. A special event was the public lecture dedicated to Lise Meitner, *Politics "RACE" and Gender: Lise Meitner and the Discovery of Nuclear Fission*, which was delivered by R. L. Sime.[3]

3) The 2002 Minerva Summer School in Blankensee, Germany, *Computational Quantum Chemistry*, which was co-organized by the LMC and C. van Wüllen, then at the Technical University of Berlin. The school enjoyed substantial student participation (about 50) from both Germany and Israel (see Figure 5). The purpose of the school was to expose junior scientists to the methods and techniques of modern CQC and to create a platform for direct communication between the German and Israeli students and scientists. German speakers at the school were: H. J. Freund, J. Gauss, J. Sauer, W. Thiel, C. van Wüllen, H. J. Werner, and H. Zipse. Among the Israeli speakers were S. Shaik (who gave three-hour talks on VB theory, which was followed by a VB tutorial), David Avnir, G. Martin, A. Stanger, U. Peskin, and R. Baer.

4) The 2004 conference, *When Experimental Chemistry Meets Quantum Chemistry*, took place at TEC, with the participation of the following speakers: P. J. Stang, W.

Figure 5. Participants in the Minerva School (2002) in Blankensee, Germany.

Thiel, H.-U. Siehl, T. Müller, A. de Meijere, P. R. Schreiner, H. Zipse, R. West, and R. Hoffmann.

5) The 2008 conference that was held at HU involved a two-day symposium with the participation of the following international speakers: T. Ziegler and F. Furche (the 2008 LML and OYGA Awardees, respectively), H. F. Schaefer, F. Hiberty, W. Thiel, G. Frenking, M. Filatov, H. Schwarz, P. R. Schreiner, R. West, S. Wolfe, J. P. Dinnocenzo, and J. M. Galbraith. All the members of the Center delivered talks too.

6) The 2009 conference, *Computational Chemistry: Bridging Chemistry and Biology*, took place at TEC with the participation of W. L. Jorgensen, A. Dreuw, J. Sauer, O. Eisenstein, S. Shaik, and K. N. Houk as speakers (see Figure 6).

Figure 6. Plenary speakers at the 2009 LMC Symposium, Technion. From left to right: K. N. Houk, W. L. Jorgensen, A. Dreuw, J. Sauer, S. Shaik, Y. Apeloig, and O. Eisenstein.

7) The 2013 LMC symposium took place at the Weizmann Institute of Science (see Figure 7). R. J. Bartlett (LML Awardee) and J. Neugebauer (OYGA) were the guest speakers.

8) The 2015 conference took place at Tel Aviv University and marked 50 Years of German-Israeli Diplomatic Relations, with the following speakers: G. E. Scuseria (LML Awardee), J. Kästner (OYGA), J. Sauer, H. Schwarz, P. R. Schreiner and W. Thiel.

4.5.2 Awards Programs

The LMC has three yearly award programs:

1) The major award of the Center is the Lise Meitner Lectureship (LML) award, given to a prominent quantum chemist who has left his/her mark on the field and the chemical community.

2) The second award, the so-called Outstanding Young German Award (OYGA), is given to young German quantum chemists below the age of 40, who have excelled in the field. This program was created for fostering German-Israeli relationship through young and bright German scientists. This has been achieved by inviting to the LMC promising young German scientists who constitute the leaders of the future scientific generation in Germany. We are pleased that many of the OYGA Awardees have already become leading researchers in CQC in Germany and in the world.

3) The third award is the Lise Meitner Junior Prize (LMJP) presented each year, during the opening ceremony of the Israel Chemical Society meeting, to the young scientist in Israel (not necessarily belonging to the

Figure 7. Participants of the 2013 LMC symposium, Weizmann Institute of Science.

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Figure 8. Lise Meitner Lecturers. From left to right: (first row) the late P. v. R. Schleyer, J. Gauss, the late J. A. Pople, R. L. Sime, K. N. Houk; (second row) H. F. Schaefer III, W. Thiel, J. Michl, L. Radom, R. Hoffmann; (third row) M. Parrinello, D. G. Truhlar, F. Weinhold, the late T. Ziegler, W. L. Jorgensen; (fourth row) S. Grimme, G. Frenking, R. J. Bartlett, G. Scuseria, and J. S. Francisco.

Center) who has written the best computational paper within the past year or so. Several of the prize recipients are now faculty members in universities in Israel and abroad.

Modes of Selection of the Awardees: The winners of the LML and the OYGAs awards are selected by a yearly ballot among the members of the Center. The LMJP award is decided by an external committee. This committee has been chaired by prominent figures in CQC: Uzi Kaldor, Amitai Halevi and Ruben Pauncz, Harlod Basch, Gernot Frenking, and presently, Gernot Frenking and Robert Berger.

The winners of the LML Award from 1998 onwards: P. v. R. Schleyer, J. Gauss (who was elected as both LML and OYGA), R. L. Sime,[3] J. A. Pople (1998 Nobel Prize Laureate), K. N. Houk, H. F. Schaefer III, W. Thiel, J. Michl, L. Radom, R. Hoffmann (1981 Nobel Prize Laureate), M. Parrinello, D. G. Truhlar, F. Weinhold, T. Ziegler, W. L. Jorgensen, S. Grimme, G. Frenking, R. J. Bartlett, and G. Scuseria. A Lise Meitner Fellow Award was bestowed on J. S. Francisco. This list of scientists encompasses the "cream" of computational chemistry leadership and covers all the major fields in computational quantum chemistry, from concepts to method development to mechanistic studies in organic, organometallic and bio-related chemistry. Figure 8 shows photos of all the Lise Meitner Lecture Awardees.

Winners of the OYGA Award: The OYGA recipients are: J. Gauss (see also Figure 8), P. R. Schreiner, H. Zipse, F. Neese, F. Furche, A. Dreuw, M. Reiher, R. Berger, J. Neugebauer, and J. Kästner. Their photos are shown in Figure 9.

Winners of the LMJP Award: The names of all the winners are given on the website of the Center.[5]

Figure 9. OYGA recipients, from left to right: (first row) P. R. Schreiner, H. Zipse, F. Neese, F. Furche, A. Dreuw; (second row) M. Reiher, R. Berger, J. Neugebauer, and J. Kästner.

5. Weaving of Scientific Ties with Science in Germany

The members of the LMC have had numerous collaborations with German scientists, in some cases extending during the entire lifetime of the Center, thus significantly strengthening the German-Israeli ties. In many cases, the scientific collaborations have developed into personal friendships which have also included the families. Here is a sample of German scientists who have collaborated with members of the Center: N. Auner (Frankfurt); R. Berger (Marburg); R. Boese (Essen); C. Bolm (Aachen); J. S. Dickschat and B. Dick (TU Braunschweig); W. Domcke (TU Munich); M. Driess (TU Berlin); T. Frauenheim (BCCMS, Bremen); G. Frenking (Marburg); S. Grimme (Bonn); M. Kaupp (TU Berlin); P. Knochel (LMU, München); S. Kümmel (Bayreuth); N. Koch (HU Berlin); U. Kleinekathofer (Jacobs University, Bremen); W. Leitner (Aachen); A. de Meijere (Göttingen); T. Müller (Oldenburg); H. Mayr (LMU, München); F. Neese (MPI, Mülheim); S. D. Peyerimhoff (Bonn); M. Scheffler (Fritz Haber Institut, Berlin); P. R. Schreiner (Giessen); the late D. Schröder (TU Berlin, Prague); D. Schülter (TU Berlin); P. v. R. Schleyer (Erlangen); H. Schwarz (TU Berlin); H. -U. Siehl (Ulm); W. Thiel (MPI, Mülheim); and H. Zipse (LMU, München).

6. Concluding Remarks

During the 18 years of its existence, the Lise Meitner Center for Computational Quantum Chemistry has accomplished a great deal, and it has even surpassed the expectations that motivated its establishment, significantly strengthening the CQC community in Israel and the German-Israeli scientific ties. The success story of the LMC shows the heights of excellence that can be achieved with a moderate size endowment and yearly interest, when there is a vision and a joint *Beirat*-directors leadership to implement the vision.

As the founders and directors of the LMC, we (S&A) feel proud of the Center's achievements and impact, and of its being a true national center for research in computational quantum chemistry. According to the rules of the Minerva Foundation, the LMC will have to be closed in 2017. It is our hope that the younger members of the Center will maintain this achievement, and create a new center that will fill in Israel the scientific vacuum created by the closure of the LMC.

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References

[1] S. S. still recalls Helmut Schwarz' assertion that Charlotte knew more about German science than any German.
[2] S. Shaik, *Isr. J. Chem.* **2015**, 55, 781–825.
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[4] a) Reprinted with permission from *Acc. Chem. Res.* **2011**, *44*, 101. Copyright 2011 American Chemical Society; b) Reprinted with permission from *J. Phys. Chem. A*, **2008**, 112, 12868. Copyright 2008 American Chemical Society; c) Reprinted with permission from *J. Phys. Chem. C*, **2013**, *117*, 22369, Copyright 2013 American Chemical Society; d) Reprinted with permission from *Soft Matter*, **2012**, *8*, 7393, Copyright 2012 Royal Society of Chemistry.
[5] The website of LMC is: http://alpha.ch.huji.ac.il/public_html/awards.htm