

## ITEM 5: SASON SHAIK

### • RESEARCH STUDENTS/POSTDOCS/ASSOCIATES:

Here is a list (ca. 80) of coworkers I have had from 1982 till now. 17 are undergraduate students, 5 graduate students, and the rest are mostly postdocs from various countries. The undergraduate and graduate students are marked in blue. The undergraduates generally completed a project and participated in a publication.

1982-1984:	Dr. E. Aharon-Shalom. Postdoctoral Fellow, Ben-Gurion University (BGU) (jointly with the Organic Metals Group: S. Bittner, J. Bernstein and J.Y. Becker).
1982-1983:	Dr. V.R. Kaufman. Postdoctoral Fellow, BGU (jointly with the Organic Metals Group).
1980-1984:	Mrs. R. Bar, Research Associate, under the auspices of Bar-Ilan University (BIU).
1982-1986:	Dr. D. Cohen, A Senior Research Associate, under the auspices of BIU
1980-1981:	Dr. J.A.R.P. Sarma. Postdoctoral Fellow, BGU (jointly with the Organic Metals Group).
1986-1988:	Ms. Avital Bartuv. An Undergraduate Research Student, BGU.
1988-1989:	Mr. Eyal Duzzi. An Undergraduate Research Student, BGU.
1989-1990:	Dr. Jeoung-Ki Cho. A Postdoctoral Fellow, BGU.
1992-present:	Dr. D. Danovich. A Permanent Research Associate, HU
1992-4:	Dr. A. Ioffe. A Senior Research Associate (emigrant from Russian), BGU (and in the Hebrew University (HU)).
1992-5:	Dr. A. C. Reddy. A Postdoctoral Fellow (The Lady Davis Fellowship), HU.
1994-6:	Dr G. N. Sastry. A Postdoctoral Fellow, HU.
1994-2000:	Ms. A. Shurki, M.Sc. and Ph.D. student, HU.
1997-2000	Dr M. Filatov. A Postdoctoral Fellow, HU
1996-7	Dr V. Dubnikov. A Senior Research Associate, HU
1997-1999	Dr. J. Galbraith. A Postdoctoral Fellow (The Lady Davis Fellowship), HU
1997-1999	Dr. N. Harris. A Postdoctoral Fellow (A Fulbright Fellowship), HU
1997-9	Dr. W. Wu, A Senior Postdoctoral Fellow, HU
1998-9	Dr. S. -J. Zhong, A Postdoctoral Fellow, HU
1999-2001	Esti Blanck, Undergraduate student, HU
1999-2000	Shimrit Cohen, Undergraduate student. HU
1999-2000	Youval Alpert, Undergraduate student, HU
1999-2002	Dr. Francois Ogliaro. A Postdoctoral Fellow (Marie-Curie Fellowship), HU
2000-2004	Dr. Samuel de Visser. A Postdoctoral Fellow, HU
2001-2002	Dr. Jose Kaneti. A Senior Postdoctoral Fellow, HU
2000-2005	Shimrit Cohen. M.Sc./ Ph.D. Student, HU
2000-2002	Dr. Pankaz K. Sharma, A Postdoctoral Fellow, HU
2001- 2004	Nir Nevo, Undergraduate student, HU.
2001- 2003	Elina Ploschnik, Undergraduate student, HU.
2002- 2005	Dr. Devesh Kumar, A Postdoctoral Fellow, HU
2001- 2007	Sebastian Kozuch, M.Sc. and Ph.D. Student, HU
2002- 2004	Avraham Gutman. Undergraduate student, HU
2002- 2004	Tamara Niazov. Undergraduate student, HU
2003-2007	Dr. K. Chazan, A Postdoctoral Fellow, HU.
2004	Dr. R. Shacham. A Postdoctoral Fellow, HU
2004-2007	Tal Katzav. Undergraduate Student, HU
2004-2007	Dr. E. Derat. A Post-Doctoral Fellow, HU
2003- 2006	E. Ploschnik. M.Sc. student, HU.
2005-2008	Dr. H. Hirao. A Postdoctoral Fellow, HU.
2005- 2009	Dr. K-B. Cho. A Postdoctoral Fellow, HU.
2006-2009	Dr. M-A. Carvajal Barba. A Postdoctoral Fellow, HU.
2006-2007	Dr. Y. Moreau. A Postdoctoral Fellow, HU.
2006-2009	Dr. C. Hui. A Postdoctoral Fellow.
2005-2009	D. Fishelovitch. A Ph.D. student, HU and Tel-Aviv U.
2007-2009	Dr. N. Jena. A Postdoctoral Fellow, HU.

2007-2010	Dr. Y. Wang. A Postdoctoral Fellow, HU.
2007-2009	R. Meir. M.Sc. student, HU
2009-2011	Dr. P. Schyman, A Postdoctoral Fellow, HU
2008-2011	Dr. W. Lai. A Postdoctoral Fellow, HU
2009-2011	Dr. D. Janardanan, A Postdoctoral Fellow, HU
2009:	J. Song. A Ph.D. student (from Xiamen, supported by the Chinese Government. for 1 year), HU.
2009:	A. Uhe. A Ph.D. student (from Univ. of Aachen, for 3 months), HU.
2009:	J. Echeverria Lopez. A Ph.D. student (from the Univ. of Barcelona, for 3 months), HU.
2009-2014:	Dr. U. Dandamundi. A Postdoctoral Fellow, HU.
2010:	M. Podewski. A Ph.D. student from the ETH (for 1 month).
2010-2011:	Dr. P. Milko. A Postdoctoral Fellow, HU
2010-2013	Dr. C. Li. A Postdoctoral Fellow, HU
2010-2012:	Dr. M. Chourasia. A Postdoctoral Fellow, HU.
2012-3:	Dr. S. Saha. A PBC Postdoctoral Fellow, HU.
2012-2016:	Dr. B. Wang. A PBC Postdoctoral Fellow, HU.
2012-3:	Dr. D. Senthilnathan. A PBC Postdoctoral Fellow, HU.
2013-2017:	Dr. D. Mandal. A Post-Doctoral Fellow, HU
2013-2017:	Dr. R. Ramanan. A PBC Postdoctoral Fellow, HU
2013-2014:	Dr. C. Wang. A Post-Doctoral Fellow, HU
2013:	J. Huang. An Exchange Student for 3 months, HU.
2014:	D. Stevens. An Exchange Student for a semester, HU
2014-2017:	Dr. Kshatresh D. Dubey. A PBC Postdoctoral Fellow, HU
2014-2017:	Dr. D. Mallick. A PBC Post-Doctoral Fellow, HU
2015-2016:	D. A. Sharon. A Fulbright Student from Princeton, HU
2015-2017:	Dr. J. Huang. A Postdoctoral Fellow, HU.
2016-2017:	Dr. S. Banda, A Postdoctoral Fellow
2016-2017:	C. J. Laconsay. A Fulbright Student from Marist College, HU
2017-2019:	Dr. Su Hao. A Postdoctoral Fellow, HU
2017-2019:	Dr. Z. Wang. A Postdoctoral Fellow, HU
2017-2018:	Dr. C.(Chao) Wang. An Exchange Ph.D. (CSC-HU exchange program) Student from the Academy of Science in Beijing, HU.
2018-2021:	Dr. T. Stuyver. A Postdoctoral Fellow, HU
2018-2021:	Dr. J. Jyothish. A Postdoctoral Fellow, HU.
2019-2020:	Dr. H. K. Kumar. A Postdoctoral Fellow, HU
2019-2021:	Dr. T. Mondal. A PBC Postdoctoral Fellow, HU.
2020-present:	Dr. N. Kuriakose. A PBC Postdoctoral Fellow, HU
2021-present:	Dr. S. Jain. A Postdoctoral Fellow, HU
2021-present:	Y. Wu. A Ph.D. Student for 1 year residence, funded by a CSC Scholarship.

## • PRESTIGIOUS RESEARCH GRANTS

In total, I have secured 52 different grants over the years 1979-2018 (the current grant will last till 2022).

**(a)** The most **prestigious** and **immensely useful grant** was the one from The Minerva Foundation in 2015 to establish a Center for Computational Quantum Chemistry. The initial funding was DM 5,150,000 (since the DM was replaced by EURO, the conversion is not straightforward, and the sum can be estimated as EUR 2,500,000 at the time of granting, plus ca. EUR 200,000 after the evaluation of the center. The proceeds of these funds can be estimated in today's currency as ca. USD 150,000/year for 20 years.

The Center was inaugurated in 1997 as "**The Lise Meitner-Minerva Center for Computational Quantum Chemistry**". It grew from 2 groups (S. Shaik in HU and Y. Apeloig in the Technion) **to a National Center with 14 groups in seven Israeli**

**Institutions, and with a world-wide reputation** (the story of the center is told in two papers: *Nachr. Chem.* **60**, 1185-1186 (2012), and *Isr. J. chem.* **55**, 1167-1176 (2015)).

**(b)** A second prestigious grant (2005-2009) is DIP (German-Israeli Project). DIP has been given yearly to very few groups (2-3) of Israeli and German scientists. Our grant involved W. Leitner, C. Bolm (from Germany), and R. Neumann and S. Shaik (from Israel). The teaming-up allowed us to tackle catalysis in general, and in particular the investigation of two-state reactivity in catalysis. One student (**A. Uhe from Aachen**) spent 3 months in Jerusalem, and participated in the new modelling of catalytic cycles which was developed in Jerusalem. **He and my Ph.D. student (S. Kozuch) wrote the AUTOF program which is now widely used.**<sup>376</sup>

**(c)** Other grants were awarded by the following agencies: ISF (1981-3; 1983-6; 1989-1991; 1996-99; 1999-2000; 2002-2005; 2006-2009; 2009-2013; 2013-2017; 2018-2022), Hebrew-University Discretionary fund (1990-1991, 1992, 1994, 2000-2001), GIF (1997-1999; 2001-2004), WOLF Foundation (1983-5), Hasselblad Foundation (1985-88), US Army (European Office, 1987-1990), VAT"AT(1995), Volkswagen (1994-6; 1997-2001), MOST (Ministry of Science and Technology, 1993), Niedersachsen (2001-2002), **Marie-Curie** (200-2001-a fellowship for Dr. F. Ogliaro), French-Israel Research Grant (2002-2005), NIH (2011-2015, in collaboration with L. Waskell), and so on.

#### • EDITORSHIP

**(a) Israel:** The Israel Journal of Chemistry (*IJC*) was established as such in the 1963 with Felix D. Bergmann being its first Editor (see, E. Keinan, S. Sarel, *Isr. J. Chem.* **50**, 8-14 (2010)). The *IJC* has gradually become the first full-fledged scientific journal of the young country, and gradually enlarged its international flavor, but suffered ups and downs, until 2009 when Editor E. Keinan managed to convince Wiley-VCH and the influential past editor of *Angewandte Chemie* (P. Göllitz) to add the *IJC* to the VCH journals. I feel very committed to the continuing survival of this journal, and hence, I have served in its editorial board from 1989 till now (with the exception of 2008, during the transition from private hands to VCH). In addition, I edited together with my colleague Apeloig, three issues in 1983, 1992 and 1993, and contributed 11 papers to the *IJC*.

**(b) Other Journals:** In addition, I have been on the editorial boards of a dozen or so journals, and am still in this capacity in a few journals (e.g., *WIREs*, *JPOC*, *JCC*, *chem<sup>2</sup>*, *Natural Sciences*); the last two are being new and promising.

**(c) Most Recent Editorial Duties (2021-2023):** Co-editing with O. Eisenstein the issues on "*Catalysis – The Land of Opportunities*" in TOPICS in CATALYSIS (by Springer). Co-Editing with P.C. Hiberty the Valence Bond Section of "Comprehensive Computational Chemistry", as part of the Multi Reference Works (MRW) initiative of Elsevier.

#### • SPECIAL NAMED LECTURES:

Here are 20 special and named lectures. I am especially proud when I am being **chosen by students** as in lectures **5** and **21**. Lecture **21** marks also the last time I spoke in front a live public (March 4, 2020) due to the pandemic.

(1) Kahlbaum Lectureship (Basel, 1988); (2,3) Troisième Cycle Lecturer (Switzerland; twice 1997, 1999 in several universities); (4) Kurt-Alder Lectureship Award (Köln, 2004); (5) The University of Minnesota Graduate-Students Lectureship (Minnesota, 2004); (6) The Charles Coulson Lectureship Award (Georgia, 2005); (7) The Christmas Lecturer (Heidelberg, 2006); (8) the IQBC Lectureship award (Prague, 2007, Academy of Sciences); (8) The Schrödinger Lecture Award (2008, Sydney); (10) L. N. Owen Lectureship (Imperial College, 2010); (11) The 1<sup>st</sup> SCILS Lecturer in Computational Science (Cape Town, 2010); (12) Frontiers in Biological Chemistry Award Lecture (Mülheim, Germany, 2012); (13) Scrocco Lectureship (Scuola Normale Superiore di Pisa, 2013); (14) Lu Jiaxi Lectureship (Xiamen, China, 2013); (15) A VIP Lecture in the 2<sup>nd</sup> International Conference on Halogen Bonding (Goteborg, Sweden, 2016); (16) Stratingh Lectureship (Groningen, Netherland, 2018); (17) The Israel Academy of Sciences Plenary Lecture in the Symposium Marking “100 Years Since the Birth of Primo Levi and 150 Years to the Publication of the Periodic Table by Mendeleev” (Israel Academy of Sciences and Humanities, 2019); (18) The Platinum Jubilee Lecture (CSIR Institute of Chemical Technology, Hyderabad, India, 2019); (19) Honorary Plenary Lecturer (The International Conference on Advanced Chemical and Structural Biology, Chennai, India, 2019); (20) The SOLVAY Colloquium (Solvay Institute, Brussels, Belgium, 2019); (21) The Van’t Hoff Plenary Lecturer, selected by a student committee (PAC Symposium, Leiden, Netherlands, 2020).

#### SELECTED AWARDS, DISTINCTIONS:

**National** Israel Chemical Society (ICS) award to outstanding B.SC. students (1971/2); ICS Medal for the Outstanding Young Chemist (1987); E. D. Bergmann Prize awarded by the Israel Academy of Sciences (1995); ICS Excellence Award (2000); Kolthoff Prize (2001); ICS Gold Medal Award (2017).

**International:** A Fulbright Fellow Award (1974-1979); Alexander von Humboldt Senior Research Award (1995-1999, 2014-2015; 2018-2019); Fellow of the AAAS (2003); included in “175 faces in chemistry” (Royal Society of Chemistry, 2012); Schrödinger Medal of the World Association of Theoretically Oriented Chemists, WATOC (2007); Frontiers in Bioinorganic Chemistry Award (2012); August-Wilhelm-von-Hofmann-Medal (German Chemical Society, 2012); Membership of the International Academy of Quantum Molecular Science (IAQMS, 2015).