

ITEM 3.

Sason Shaik: Short Curriculum Vitae (Oct-04-2021)

SHAIK PERSONALIA:

Born in Baghdad, Iraq, on 01-09-1947.

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EDUCATION:

B.Sc. (1972, Bar-Ilan University), M.Sc. (1974, Bar-Ilan University, M. Albeck), Ph.D. (1977, Seattle, the Univ. of Washington, N.D. Epiotis); Postdoc (1978, Cornell, R. Hoffmann).

ACADEMIC POSITIONS/TITLES:

Academic Positions: Lecturer, Ben-Gurion University (October 1979-1980), Sr. Lecturer, Ben-Gurion University (1981-4), Associated Professor, Ben-Gurion University (1984-1988), Professor, Ben-Gurion University (1988-1992); Professor, Hebrew University (1992-2017), Professor Emeritus (October 2017-present).

Other Academic Titles: Director of the Lise Meitner-Minerva Center for Computational Quantum Chemistry (1997-2017).

Chair Title: Saerree K. and Louis P. Fiedler Professor (2013-present).

Visiting Professorships: Université de Paris-Sud, Orsay, France (1985 (Sabbatical), 2016); Université Paul Sabatier, Toulouse, France (1986, a short course on VB theory)); Queen's University, Kingston, Canada (1986 (Sabbatical)); University of Alabama, Huntsville, USA (1986), University of Goteborg, Goteborg, Sweden (1989 (a short course on VB theory)); University of Lund, Lund, Sweden (1989 (a short course on VB theory)); University of Rochester, Rochester, USA (1996 (Sabbatical & graduate course on VB theory)); The Technical University of Berlin, Germany (1997-1999; 2014-2019 (Alexander von Humboldt Fellow) (among other activities, gave twice a short course on VB theory)); Ecole Normale Supérieure, Paris, France (2001); KTH Royal Institute of Technology, Stockholm, Sweden (2007 (a short course on VB theory)); Ewha University, Seoul, Korea (2008, 2009), University of Xiamen, Xiamen, China (a few times during 2011-2019); Pierre and Marie Curie University, Paris, France (2015).

Selected Short-Terms Visits and Lecture Series: France (often; 1984-2015); USA (often: 1986-2014); Italy (1987, 2013); Switzerland (1988, 1997, 1999); Spain (1988, 2000, 2004, 2011, 2012, 2018); Sweden (1989, 1996, 2007); Austria (1998, 2010); South Africa (2005, 2010); China (often, 1999-2018); Taiwan (2003); Czech Rep. (2007); Australia (2008); Germany (often; 1993-2019); India (2005, 2019); Singapore (2013); Netherlands (2018, 2020); Belgium (2019).

AWARDS, DISTINCTIONS:

Named Lectures: Kahlbaum Lectureship (Basel, 1988); Troisième Cycle Lecturer (Switzerland; twice 1997, 1999); Kurt-Alder Lectureship (Köln, 2004); Minnesota Graduate-Students Lectureship (Minnesota, 2004); Charles Coulson Lectureship (Georgia, 2005); Christmas Lecturer (Heidelberg, 2006); IQBC Lectureship (Prague, 2007, Academy of Sciences); Leonard N. Owen Lectureship (Imperial College, 2010); the 1st SCILS Lectureship Series in Computational Science (Cape Town, 2010); Scrocco Lectureship (Scuola Normale Superiore di Pisa, 2013); Lu Jiaxi Lectureship (Xiamen, China, 2013); Stratingh Lectureship (Groningen, Netherland, 2018); Platinum Jubilee Lecturer (CSIR Institute of Chemical Technology, Hyderabad, India, 2019); Honorary Plenary Lecturer (The International Conference on Advanced Chemical and Structural Biology, Chennai, India, 2019); SOLVAY Colloquium Lecturer (Solvay Institute, Brussels, Belgium, 2019); Van't Hoff Lecture (PAC Symposium, Leiden, Netherlands, 2020).

Selected Awards and Distinctions:

National: Israel Chemical Society (ICS) Prize for Undergraduate Students (1971/2); the ICS Medal for the Outstanding Young Chemist (1987); E. D. Bergmann Prize (1995); The ICS Excellence Award (2000); The Kolthoff Prize (2001); The ICS Gold Medal (2017).

International: Fulbright Fellow Award (1974-1979); DAAD Fellow (1980); NSERC (National Research Council of Canada) Exchange Award (1985); 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 Chem. Soc., 2012); Membership of the International Academy of Quantum Molecular Science (IAQMS, 2015).

PUBLICATIONS:

ca. 590, including 4 books and 3 edited-books, 30 reviews & book chapters, and 12 essays. Citations (Google Scholar/[ISI]): 44,240/[37,940], H-index = 105/[96].

Among the papers 209 are in leading journals: 136 papers in *J. Am. Chem. Soc.*; 45 papers in *Angew. Chem. Int.*; 28 papers in *Acc. Chem. Res.*, *PNAS*, *Nat. Chem.*, *Nat. Commun.*, *Cell Press (Chem., & Trends in Chemistry)*.

CONFERENCES:

Plenary, Keynote, invited (including named and award lectures): ca-330.

MENTORING:

I mentored ca-80 undergraduate research students, M.Sc./Ph.D. students, and postdocs.

ORGANIZATION OF MEETINGS:

As a director of the Lise Meitner-Minerva Center, I organized in Jerusalem 18 Conferences with **International and Israeli Speakers**. I was a member of Organizing Committees in numerous other conferences.

BOARD MEMBERSHIPS:

Member of the Advisory Board of WATOC (1998-present); Member of the Assembly of IAQMS (2015-present); Member of the European Committee on the Chemical Bond, ECCB (2018-present).

SELECTED UNIVERSITY DUTIES:

Chaired the Computing and Communication Committee of the Faculty of Natural Sciences and Mathematics (1998-2000); Member of the Computing and Communication Authority of the Hebrew University (1998-2000); Head of the Institutional Selection Committee of New Recruits (2003-2009); Head of the University-Wide Committee for the Promotion to the Rank of Full Professor in the Experimental Sciences, Computer Science and Mathematics (2010-2014).

SELECTED EDITORIAL BOARDS AND EDITORSHIP DUTIES:

Member of the editorial board of the Israel Journal of Chemistry, IJC (1989-present); Member of the editorial board of the Journal of Computational Chemistry, JCC (2001-present), Member of the editorial board of the Journal of Physical Organic Chemistry (2005-present), Member of the international advisory board of Wiley Interdisciplinary Reviews, WIREs (2008-present); Advisory board member of Wiley's new interdisciplinary Journal *Natural Sciences* (2021-present); Board member of the new Journal of Chemistry Supporting Chemists, *Chem²* (2021-present); Was on the advisory boards of THEOCHEM, Theoretical Chemistry Accounts, Journal of Inorganic Biochemistry (1995-2009); co-Editor (with P.C. Hiberty) of **the Valence Bond Section** of "Comprehensive Computational Chemistry", as part of the Multi Reference Works (MRW) initiative of Elsevier (2021-present); co- Editor (with O. Eisenstein) of the issues on "*Catalysis – The Land of Opportunities*" in TOPICS in CATALYSIS (by Springer).

REACHING OUT:

- **Taught gifted children** (1972-1973).
- **Was the Academic Advisor** to "*The Unit for the Education of Gifted Children*" (1989-1991).
- **Was a council member** of "*The Association for the Promotion of Research, Literature and Art*" (founded by Iraqi Jews).
- **Was a member** of the "*Committee for the Advancement of Humanities in Israel*" (2017-2019).
- **Gave numerous public lectures** to general audience, high school students, as well as to chemists, about Chemistry Being a "*Central Pillar of Human Culture*", about History of Chemistry in Israel, and the Periodic Table (Mendeleev, Primo Levi, etc.).

- **Wrote a book of chemistry to a general audience:** *Chemistry as a Game of Construction: The Bond-Click Way* (Wiley, 2016) based on a course given to humanities and social science students. The book introduces **a new way of teaching chemistry**.
- Wrote on the **History of Establishing Chemistry in the Hebrew University (1923) and in Israel** ("A Tale of Two Mounts: The History of Chemistry at the Hebrew University of Jerusalem", *Isr. J. Chem.* **55**, 781-825 (2015)).
- **Taught History of Chemistry** between 2009-2017 and will be doing this again in 2022.
- **Taught** a Course of "**Chemistry as a Game of LEGO**" to **humanities and social science** students (1992-1995; 1997-8; 2019-2017).
- Wrote **essays on chemistry and history**: 12.
- 1997-2017: Directed **The Lise Meitner-Minerva Center for Computational Quantum Chemistry** (with co-Director Y. Apeloig). During this time span the center evolved from two groups in two institutions, to **a National Center with international repute**.
- Participated in the **Malta Conferences** which Bring Together Arab and Israeli Scientists.
- Wrote/Write poetry (some on matter and mind) and essays.

KEY SCIENTIFIC CONTRIBUTIONS:

Sason Shaik is a chemical theorist who has contributed to the intellectual fabric of chemistry new concepts and paradigms that create generalities, elucidate known phenomena and make verifiable predictions on unknown phenomena:

(a) His initial work²⁴ in 1981, and work that followed, have been responsible for the renaissance of Valence Bond (VB) theory, in which he developed a general model for chemical reactivity in terms of just two VB diagrams (one for single step reaction, the other for stepwise reactions). In so doing, he contributed to a unified understanding of reactivity, and provided the tools for making new predictions of numerous phenomena, from organic to organometallic chemistry and enzymes. **See highlights.**

(b) A subsequent work⁴² in 1984, and work that followed, have changed completely the understanding of icon molecules like benzene (& other aromatic molecules) and allylic species, by showing that the delocalized π -electrons of these species are unstable transition states, which are trapped within rigid σ -frames that enforce the uniform bond lengths of these molecules. These predictions were later found proves in spectroscopy (1995-7^{124,126,127}). **See highlights.**

(c) He developed new models of chemical bonding (called **charge-shift bonds** with Hiberty, and **triplet pair bonds**), which are changing the mental map of the Chemical Bond. **See highlights.**

(d) His work in the mid-1990s¹²¹ (with Schwarz) formulated the phenomena of single-state reactivity (SSR) vs. two-state reactivity (TSR), which has become a central pillar in oxidative chemistry ranging from small molecules (like FeO^+) all the way to metallo-

enzymes such as Cytochrome P450. The TSR paradigm changed the way bioinorganic chemists design and interpret their experiments. **See highlights.**

(e) His articulation (2010-2011)^{361,380} of the concept of exchange-enhanced reactivity (EER) introduced a new and hitherto unrecognized factor that controls energy barriers (the exchange interaction between identical spins on the same center). **EER accounts for the choice of nature to select metallo-enzymes with high-spin species.**

(f) Recently (2004-2021)^{248,479,530,585} he **pioneered** the development of the area of using oriented external and local electric fields (OEEFs, LEFs) for **control of reactivity, selectivity, asymmetric catalysis, and structure. See highlights.**

(g) Among other contributions are: (1) the recognition of **entangled reactivity** in mechanisms which involve the same set of VB structures, and which possess **a single transition state that serves two different products**^{128,134,149} (section 9.3.3 in paper 149). (2) The quantitative modelling of catalytic cycles and derivation of the turnover frequency (TOF) of the catalysis.^{376,377}

EXAMPLES OF INCORPORATION OF WORK INTO TEXTBOOKS & HIGHLIGHTS OF WORK:

THE VB WORK (18981-on):

(a) The VB work was characterized by R. Hoffmann (R. Hoffmann, *Chemistry in Britain*, March 1991, Letters section) as a main contribution to the renaissance in valence bond theory.

(b) The VB model has been incorporated into leading text books: (1) T.H. Lowry, S. Richardson, "*Mechanism and Theory in Organic Chemistry*", 3rd Ed 1987 (introductory page xi, and pp 218-223, 229, 354-360, 371, 381-382, 412, 604-608, 659, 685, 769). (2) F. A. Carroll, "*Perspectives on Structure and Mechanism in Organic Chemistry*", Brooks/Cole Publ Co 1998 (pp. 213, 227, 265, 301, 497, 506-511, 740, 879). (3) L. Eberson, "*Electron Transfer Reactions in Organic Chemistry*", 1987 (on p. 8 (the model is introduced as "*An alternative to the Marcus model...*"); other usages of the VB model: pp, 23-25, 95, 141-142, 193. (4) The VB modeling of bonded ET was reviewed in the highlight section of *Angewandte Chemie Int. Ed.* by: H. Zipse, *Angew. Chem. Int. Edit. Engl.* **1997**, 36, 1697.

THE NEW STORY OF BENZENE AND OTHER DELOCALIZED SPECIES (1984-on):

(a) The work has been chosen as one chapter of a total of 17 written as a dialogue between a young and an old scientist on the status of the theory of chemical bonding "the same way Hume-Ruther's characters did [in their dialogue]". J.K. Burdett, "*Chemical Bonding A Dialog*", 1997 (Chapter 12: "*Is Delocalization of Electrons Always Stabilizing? Or, Why is Benzene a Regular Hexagon?*").

(b) The work was highlighted in: (1) C&EN, Nov. 3, 1997 in Science and Technology Concentrates. (2) CHEMTRACTS: J. K. Burdett, *CHEMTRACTS- INORGANIC CHEMISTRY*, **1991**, 3, 57-61. (3) Highlighted by E. Heilbronner, *J. Chem. Ed.* **1989**, 66, 471 (4) Reviewed by J.J.C. Mulder, *J. Chem. Ed.*, **1998**, 75, 594. (5) Reviewed by the Historian of chemistry, S.G. Brush, "*Dynamics of Theory Change in Chemistry: The Benzene Problem*": *Studies in History and Philosophy of Science*, **1999**, 30, 21; **1999**, 30, 263.

(c) The work has been incorporated into Textbooks: (1) in: F. Carroll, "*Perspectives on Structure and Mechanism in Organic Chemistry*", 2nd Ed., 2010, e.g. p. 250. (2) In an advanced monograph on aromaticity: P.J. Garrat, "Aromaticity", Wiley, 1986. (3) In V. Minkin, V.; B. Simkin, B.; M. Glukhovtsev, "Aromaticity and Antiaromaticity", Wiley: New York, 1994.

TWO-STATE REACTIVITY:

(a) Highlighted in: (1) D.A. Plattner, *Angew. Chem. Int. Edit. Engl.*, **1999**, 38, 82-85. (2) *Chemistry and Chemical Industry*, **2001**, 54-6, 680 (the Japanese equivalent of *Chem. Eng. News*). (3) P.R. Ortiz de Montellano, J.J. de Vos, *Nat. Prod.* **2002**, 19, 477-493, write about the two-state reactivity work: "*This mechanism is at once as complex, intriguing and satisfying as the chemistry of the P450 enzymes themselves*", and ends his review article in the following statement: "*Perhaps one of the most useful advances in the recent past has come from computational chemistry, which has provided a two-state reactivity model that readily rationalizes the experimental data*".

NEW BONDING TYPES

(a) (1) The work on charge-shift bonding (CSB) was discussed twice in C&E News (C&E News in January 29, 2007, pp 37-40, Volume 85, Number 05; C&E News, May 11, 2009, pp. 32). (2) CSB was highlighted in 2002: A New Type of Bond: Charge Shift Bonds", S. Shaik, P.C. Hiberty, 2020, *Adv. Sci. News*, July 3, <https://www.advancedsciencenews.com/a-new-type-of-bond-charge-shift-bonds/> "A newly discovered class of fundamental bonding interactions is changing our understanding of chemistry". (3) The work on quadruple bonding in C₂ was highlighted in *Comput. Chem. Highlights*, and twice in *Chemistry world* (<http://www.rsc.org/chemistryworld/News/2012/January/carbon-carbon-quadruple-bond.asp>); Philip Ball, "*the Name's Quadruple Bond*", May 13, 2013. (4) The work on bonding was reviewed in *Chemistry world* pp. 50-54, February 2014, by Philip Ball, "*What's a Bond?*"

ELECTRIC FIELD EFFECTS ON REACTIVITY AND STRUCTURE

(a) (1) 2018 (09 January): A feature article in *Chemistry World* by J. Howgego, "*Field of Influence*" [<https://www.chemistryworld.com/feature/can-we-control-reactions-with-electric-fields/3008354.article>]. (2) B. Halford, "*Zapping Diels-Alder reactions: Electric Field Spurs Reagents to Join Up in Nonredox Transformation*". C&EN, March 7, 2016.

(2) K. Krämer, "*Electric Field Flicks Switch for Bond Breaking Reaction*", *Chemistry World*, 28 June 2019. (3) A. Extance, "*Electrostatic Field Powers Up Reaction Rate*", *Chemistry World*, 2 March 2016. (4) G. Li, "*Electric Chemistry*", *New Scientist*, 15 August 2020, 45-47.