

SASON SHAIK (SASON S. SHAIK)

CURRICULUM VITAE

FEBRUARY 2021

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1. PERSONAL DETAILS

Name: Sason Shaik

Birth: Baghdad, Iraq

Immigration: March 1951 (to Israel)

Military Service: 1965-1968 (IDF)

University Address: The Institute of Chemistry
The Hebrew university
91904 Jerusalem, Israel
Tel: 972-2-6585909, FAX: 972-2-6585345

Home Address: H'namer St 7/3
Jerusalem 96954, Israel
Tel: 972-2- 6782964

2. EDUCATION

B.Sc.: 1968-1972, Bar-Ilan University, Department of Chemistry, *summa cum laude*.

M.Sc.: 1972-4, Chemistry, Adviser: M. Albeck, Thesis: "Reactions Between Halides of Te(IV) and Unsaturated Hydrocarbons", with excellence.

Ph.D.: 1974-1978, University of Washington, Department of Chemistry. Adviser: N.D. Epiotis, Thesis: "Spin Inversion in Triplet Reactions".

Post Doctoral: 1978-1979, Cornell University, Department of Chemistry. With Roald Hoffmann

3. EMPLOYMENT HISTORY

1972-1974: Teaching Assistant, Bar-Ilan University.

1972-1973: Teacher, Bar-Ilan University, teaching gifted children.

1974-1978: Teaching Assistant, The University of Washington.

1980: Lecturer, Ben-Gurion University

1980-1984: Senior Lecturer, Ben-Gurion University.

1982: Senior Lecturer (tenured), Ben-Gurion University

1984-1988: Associate Professor, Ben-Gurion University.

- 1984-1985: Visiting Foreign Scientist, Université de Paris-Sud
 1985: Visiting Professor, Queen's University
 1988: Professor, Ben-Gurion University
 1992-present: Professor, The Hebrew University

4. PROFESSIONAL FUNCTIONS

(A) EDITORSHIP AND ADVISORY DUTIES

- 1983: Guest Editor of the Israel Journal of Chemistry (the Special Issue on "Applications of Theory to Organic and Organometallic Molecules", Part 1 of Vol 23, 1983, jointly with Y.Apeloig).
- 1992/3: Guest Editor of the Israel Journal of Chemistry (the 1992 Wolf Prize Special Issue, entitled, "Computational Quantum Chemistry-- A Cornerstone of Chemical Research", Parts 3 and 4 of Vol 33, 1993, jointly with Y.Apeloig).
- 1989- present: Member of the Editorial Board, The Israel Journal of Chemistry.
- 1994-1996: Member of the International Megalon Chemistry Advisory Board (MEGALON S.A., Switzerland).
- 1995-present: Member of the Editorial Board, THEOCHEM.
- 2001- present: Member of the Editorial Board, Journal of Computational Chemistry.
- 2002-: Member of the Editorial Board, Theoretical Chemistry Accounts.
- 2005-present: Member of the Editorial Board, Journal of Physical Organic Chemistry.
- 2005-: Member of the Editorial Board, Journal of Inorganic Biochemistry.
- 2008-: Member of the International Advisory Board, Wiley Interdisciplinary Reviews.
- 2009-present: Member of the International Advisory Board of the 'State Key Laboratory of Physical Chemistry of Solid State Surfaces', in the University of Xiamen, Xiamen, China.
- 2010-: Member of the Editorial Board of the Israel Journal of Chemistry (in its new Wiley-VCH home).
- 2015-: Member of the Editorial Board of the Dutch Journal of Chemical Technology, (<http://www.lectitojournals.com/dutch-journal-of-chemical-technology>)
- 2020-: Member of the Advisory Board of *Natural Sciences*

(B) ORGANIZING COMMITTEES OF SYMPOSIA AND MEETINGS

- 1982: Member of the organizing committee of the Fourth International Symposium on Inorganic Ring Systems (IRIS).

- 1986: Member of the organizing committee of the Fifth ESOC Conference.
- 1986: Member of the organizing committee of the Symposium of Molecular Electronics (organized by the Committee of Research and Development in the Ministry of Science and Development).
- 1994: Member of the organizing committee of the 1994 Italo-Israeli Symposium on Physical Organic Chemistry.
- 1994: Member of the organizing committee of the 1996 WATOC Symposium.
- 1997-8: Member of the organizing committee of the 1998 Italo-Israeli Symposium on Physical Organic Chemistry.
- 1998-9: Member of The International Advisory Board, WATOC'99
- 1998-2000: Member of The International Advisory Board, ICPOC' 2000
- 2002: Member of the Advisory Board of WATOC
- 1997-2016: Organized 18 Lise Meitner International Symposia of the Lise Meitner-Minerva Center for Computational Quantum Chemistry.
- 2008-9: Member of the Organizing Committee of ESOR 12 (the 12th European Symposium on Organic Reactivity).
- 2008-11: Member of the Organizing Committee of Malta IV (Science and Education in the Middle East).
- 2011: Member of the International Advisory Board for WATOC 2011
- 2011: Member of the International Advisory Board for ATOMS 2011 (Hyderabad)
- 2012-3: Member of the Organizing Committee for the 2nd EuChems Inorganic Chemistry Symposium, Jerusalem, 2013.
- 2012 Member of the Organizing Committee of the 1st Valence Bond Workshop in the Université Pierre et Marie Curie, Paris 06, France [see: *ChemPhysChem* **2012**, *13*, 4029 – 4030]
- 2015-2018 Member of the Organizing Committee of the 2nd -4th Valence Bond Workshops in the University of Xiamen, China; Aachen, Germany (CB2017) & Marseilles, France (VALBO-1).

(C) ACADEMIC ADMINISTRATION

- 1980-1991: Departmental representative on the Library Committee, Ben-Gurion University (with the exception of 1984 and 1985: on Sabbatical and a Leave of Absence).

- 1982-1991: Member of the Departmental Undergraduate Studies Committee, Ben-Gurion University (with the exception of 1984 and 1985: on Sabbatical and a Leave of Absence).
- 1989-1991: Academic Adviser to the Unit for the Education of Gifted Children.
- 1991-present: Council Member, "The Association for Promotion of Research, Literature and Art (founded by Jews from Iraq)".
- 1992-1995: Member of the Tenure Committee in the Experimental Sciences in the Hebrew University.
- 1991-2000: Member of the IUPAC Working Party on "Glossary of Terms in Theoretical Organic Chemistry".
- 1992-4: Member of the IUPAC Working Party on History of Chemistry in Europe.
- 1996-2000: Member of the Promotion Committee in the Experimental Sciences in the Hebrew University.
- 1997: Member of the Research Committee in the Experimental Sciences in the Hebrew University.
- 1997-2017: Director of the Lise-Meitner Minerva Center for Computational Quantum Chemistry.
- 1998-2000: Chairman of the Computing and Communication Committee of the Faculty of Natural Sciences.
- 1998-2000: Member of the Computing and Communication Authority of The Hebrew University.
- 2001-2007: Member of the Institutional Promotion Committee.
- 2005-2008: Elected Senator; representative of the faculty of sciences in the Senate.
- 2003-2009: Head of the Institutional Selection Committee.
- 2010-2014: Head of the University-wide Committee for Promotion to the Rank of Full Professor in the Natural Sciences and Mathematics.
- 2017-present: Member of the Committee for the advancement of Humanities in Israel, Established by the Council for Higher Education.

5. PLENARY / INVITED LECTURES

A selection of talks is listed below (NOT included *approx.* 250 departmental and center seminars):

- (1) 1981: An Invited Talk
"On the Origins of the Barrier in S_N2 Reactions"
The 47th Israel Chemical Society Meeting
Beer Sheva, Israel.
- (2) 1983: An Invited Talk
"Conceptualization and Design of New Organic Metals"
Symposium on the Physics of Polymers and Macromolecules
Weizmann Institute of Science, Rehovot, Israel.
- (3) 1983: An Invited Talk
"Strategic Design of Organic Conductors. Structure of a Prototypical Molecule"
The 4th Gentner Symposium on Organic Materials with Special Physical Properties
Ginosar, Israel
- (4) 1985: An Invited Talk
" S_N2 as a Single Electron Transfer Reaction. TS Geometries and their Relationship to Other Reactivity Features"
190th National ACS Meeting, Chicago, USA.
- (5) 1985: A Plenary Lecture
"The Relationship Between S_N2 and Single Electron Transfer Stepwise Mechanisms. A Theoretical and Experimental Overview"
Midwest ACS Regional Meeting, Carbondale, Illinois
- (6) 1985: **Invited Series of Lectures** (under the auspices of French Chemical Society)
"The Collage of S_N2 Reactivity. An Overview"
Universite Paul Sabatier, Toulouse, France.
- (7) 1986: **Invited Series of Lectures**
"Chemical Reactivity. An Overview"
University of Alabama, Huntsville, Alabama, USA.
- (8) 1986: An Invited Talk
"Electronic Delocalization is Not a Driving Force in Organic Chemistry"
The 52nd Israel Chemical Society Meeting
Ramat Gan, Israel.
- (9) 1986: **Invited Series of Lectures**
"Organic Conductors"
Consortium for Materials Development in Space
University of Alabama, Huntsville, Alabama, USA.
- (10) 1986: A Plenary Lecture

"Strategic Design of EDA Organic Conductors"
Israel Scientific Conferences. Symposium on Molecular Electronics. The
National Council for Research and Development.
Jerusalem, Israel.

- (11) 1987: An Invited Talk
"Electron Delocalization is not a Driving Force in Organic Chemistry"
Swedish-Israeli Symposium on "New Trends in Organic Chemistry"
The Weizmann Institute of Science, Rehovot, Israel.
- (12,13) 1987: Two Plenary Lectures
"Chemical Reactivity"
The Symposium on Understanding of Chemical Reactivity
Centre National de la Recherche Scientifique (CNRS)
Pouilly-Sur-Loire, France.
- (14) 1987: An Invited Talk
"Organic Metals and Their Isomeric Charge Transfer Complexes"
The Italian-Israeli Joint Symposium On Solid State Chemistry.
Florence, Italy.
- (15) 1987: **Invited Series of Lectures**
"A Search for Significance in Chemical Reactivity"
The University of Padova
Padova, Italy.
- (16-20) 1988: **Invited Series of Lectures (5 hours) as a Plenary Speaker**
"A Qualitative Valence Bond Approach to Organic Reactions"
The NATO Summer School on "New Theoretical Concepts for Understanding
Organic Reactions".
San-Feliu De Guixoles, Spain
- (21) 1988: **The Kahlbaum Lectureship**
The University of Basel
Basel, Switzerland.
- (22) 1989: A Plenary Lecture
"The LEGO Way: Curve Crossing Diagrams as General Theoretical Models
for Chemical Reactivity and Structure".
The 54th Israel Chemical Society Meeting
The Weizmann Institute of Science, Rehovot, Israel.
- (23-28) 1989: **Invited Series of Lectures**
"The LEGO Way: Curve Crossing Diagrams as General Theoretical
Models for Chemical Reactivity and Structure".
University of Goteborg
Goteborg, Sweden.
- (29-34) 1989: **Invited Series of Lectures**
"The LEGO Way: Curve Crossing Diagrams as General Theoretical
Models for Chemical Reactivity and Structure".
University of Lund
Lund, Sweden.

- (35) 1989: A Section Main Lecture
" A Search for Significance. Reactivity Patterns in Reactions between Electrophiles and Nucleophiles".
The 32nd IUPAC Congress
Stockholm, Sweden
- (36) 1989: A Section Main Lecture
" When Does Electronic Delocalization Become a Driving Force of Chemical Bonding and Structure?".
The 6th ESOC Conference
Belgrade, Yugoslavia.
- (37) 1989: A Plenary Lecture
" VB Theory in Organic Chemistry".
The SECAM Symposium for Planning a Meeting on VB Theory.
Centre Europeen de Calcul Atomique et Moleculaire (CECAM),
Orsay, France.
- (38) 1990: A Plenary Lecture:
"The LEGO Way: Curve Crossing Diagrams as General Theoretical Models for Chemical Reactivity and Structure".
The 10th IUPAC Symposium on Physical Organic Chemistry
Haifa, Israel.
- (39) 1990: A Plenary Lecture:
" The LEGO Way: Curve Crossing Diagrams as General Models in Physical Organic Chemistry".
The SECAM VB Workshop.
Centre Europeen de Calcul Atomique et Moleculaire (CECAM),
Orsay, France.
- (40) 1990: A Plenary Lecture
"Valence Bond Curve Crossing Diagrams as General Models for Chemical Reactivity and Structure"
The 1990 EUCHEM Conference on "Theoretical Chemistry and Organic Synthesis".
Cavaillon, France.
- (41) 1990: An Invited Talk
"Curve Crossing Diagrams as General Models for Chemical reactivity and Structure."
The First Japan-Israel Conference on Molecular Science.
The Hebrew University, Jerusalem, Israel.
- (42) 1991: A Section Main Lecture
"Single Electron-Transfers, -Shifts, and -Enforced Transfers in Electrophile-Nucleophile Reactions of Even- and Odd-Electron Reactants"
The ACS National Meeting, Atlanta (the Symposium on Single Electron Transfer Initiated Reactions).
Atlanta, USA.
- (43) 1991: A Plenary Lecture
" Valence Bond Mixing in Organic Chemistry: The "LEGO" Way".

The VIIth International Symposium of Quantum Chemistry.
Menton, France.

- (44) 1991: A Plenary Lecture
"Electron Transfers and Nucleophilic Cleavages of One Electron σ -Bonds".
The Electron Transfer Symposium (a Satellite of the VIIth International Symposium of Quantum Chemistry).
Sophia Antipolis, France.
- (45) 1991: An Invited Lecture
"Electron Transfers and Nucleophilic Cleavages of One Electron σ -Bonds".
The Third European Symposium of Organic Mechanisms (ESOR III)
Goteborg, Sweden.
- (46-56) 1991, 1996: **Invited Series of Lectures**
1991: "Valence Bond Paradigms in Reactivity and Structure".
1996: "Valence Bond Theory"
The University of Rochester, Rochester, NY, USA.
- (57) 1992: A Plenary Lecture
"Valence Bond Mixing in Organic Chemistry: The "LEGO" Way".
The 2nd Italian-Israeli Symposium on Stereoelectronic Effects.
Herzlia, Israel.
- (58) 1992: An Invited Lecture
"ET vs Polar Mechanisms. Transition State Structures and Properties for Reactions of Cation Radicals and Nucleophiles."
The 57th Israel Chemical Society meeting
Haifa, Israel.
- (59) 1992: An Invited Lecture
"Transition State Structures of Electron Transfer Reactions: Are They Really Outer-Sphere ?"
The Joint Symposium of The Israel Academy of Sciences and Humanities and The Royal Swedish Academy of Sciences, on:
"100 Years of The Arrhenius Rate Law"
Jerusalem, Israel.
- (60) 1992: A Plenary Lecture
"Cation Radicals and Nucleophiles: Reactivity Patterns"
The Gordon Conference of Ion Radicals.
- (61) 1993: An Invited Lecture
"A Look at Transition States of Electron Transfer Reactions of Organic Species"
Second Joint Symposium, The Hebrew University of Jerusalem and The Free University of Berlin,
"Light Induced Processes in Molecular Assemblies."
Jerusalem, Israel
- (62) 1993: A Plenary Lecture

"A Look at Mechanisms of Electron Transfer Reactions of a Cation radical and Nucleophiles".
4th Annual Symposium for "Photoinduced Charge Transfer".
The University of Rochester
Rochester, NY, USA.

- (63-64) 1993: **An Invited Series of Lectures**
"Valence Bond Paradigms in Chemical reactivity and Structure"
The Technical University of Berlin
Berlin, Germany.
- (65) 1993: A Plenary Lecture
"Avoided crossing States, Transition States and Valence Bond Mixing:
Fundamental Reactivity Paradigms".
The 29 Faraday Symposium on "Potential Energy Surfaces".
The Royal Society
Oxford, England.
- (66) 1994: An Invited lecture
"Single Electron Shifts and Avoided crossing States: Fundamental Paradigms in
S₂ Reactivity".
207th ACS National meeting
San Diego, CA, USA.
- (67) 1994: A Plenary Lecture
"Perfectly Resonating States and Valence Bond mixing: Fundamental
Reactivity Paradigms".
The 25th Reaction mechanisms Conference
Notre Dame, Indiana, USA.
- (68) 1994: An Invited Lecture
"Perfectly Resonating States and Valence Bond mixing: Fundamental
Reactivity Paradigms".
The 1st Italy-Israel Symposium on Physical Organic Chemistry.
Sassari, Italy.
- (69) 1994: An Invited Lecture
"What is a Good Approximation for the Transition State of a Chemical
Reaction?"
The 2nd Swedish-Israeli Symposium on New Trends in Organic Chemistry.
Stockholm, Sweden
- (70) 1994: An Invited Lecture
"The Perfectly Resonating State. A Fundamental Model for the Transition State
of a Chemical Reaction".
The 2nd Chinese-Israeli Meeting on reaction Dynamics and Laser Chemistry.
The Academy of Sciences, Jerusalem, Israel.
- (71) 1995: An Invited Lecture
"Selection Rules for Electron transfer and Substitution Reactions of Anion
Radicals".
The 60th Israel Chemical Society meeting, Rehovot, Israel.
- (72) 1995: An invited Lecture

"Structure and Bonding principles in Electron Transfer Transition States and Their Bond Forming Analogs. Orbital Selection Rules."
 The 3rd Joint Symposium of the Technische University of Berlin and the Hebrew University of Jerusalem.
 Berlin-Brandenburgische Akademie der Wissenschaften, Germany

- (73) 1995: An Invited Lecture
 "Structured Electron Transfer Transition States for Reactions of Anion Radicals and Alkyl Halides. Selection Rules."
 25th North Eastern Regional meeting, American Chemical Society, Rochester, USA.
- (74) 1996: A Plenary Lecture
 "To be or not to be Delocalized is the Question: A different Story of Benzene, Allyl, and Delocalized Species".
 WATOC Symposium, Jerusalem, Israel.
- (75) 1996: A Plenary Lecture
 Electron Donor Acceptor Interactions
 "Transition States for Organic Electron transfer Reactions"
 The Gordon Conference in Newport, Rhode Island, USA.
- (76) 1997: An Invited Lecture
 IX International Congress on Quantum Chemistry
 "Two-State Reactivity in the Mechanism of H-H/C-H Bond Activation by Metal Oxenide Cations."
 Atlanta, Georgia, USA
- (77) 1997: An Invited Lecture
 The Israel Chemical Society Annual Meeting
 "Two-State-Reactivity in the Mechanism of C-H Bond Activation by Metal Oxenide Cations."
 Haifa, Feb. 1997
- (78) 1997: A Plenary Lecture
 ESOC-10
 "Two-State Reactivity in the Mechanism of C-H Bond Activation by Metal Oxenide Cations."
 European Symposium of Organic Chemistry, Basel, Switzerland
- (79) 1997: A Plenary Lecture
 33rd Symposium on Theoretical Chemistry of German Speaking Chemists
 "A Kekule Crossing Model: What Can We Learn on the Behavior of the π -Electrons in the Ground State of Benzene and other Conjugated Systems from the Exalted Frequencies of the Localizing Modes in the Covalent Excited States."
 Cologne (Walberberg), Sept. 1997.
- (80-84) 1997: **Troisieme-Cycle Lecturer**
 A series of 5 Lectures
 VB paradigms, TSR, ET, Benzene Story
 Fribourg, Berne, Geneve; Sept.-Oct. 1997

- (85-88) 1998: **Lecturer of the Austrian Chemical Society**
A series of 4 Lectures
Electron transfer reactivity, P-450 Activation, a different story of Benzene
Vienna, Innsbruck and Graz, May 5-15, 1998
- (89) 1998: Invited Talk
The 2nd Israeli-Czechia Meeting on Molecular Dynamics
The Israel Academy of Sciences, Jerusalem, May 3-5, 1998
- (90) 1998: Plenary Lecture
“Some Attempts to Marry VB and DFT Theories”
The 1st Israeli Symposium on “Frontiers in Electronic Structure Calculations”
The Lise Meitner-Minerva Center and The Advanced Study Institute of
Theoretical Chemistry (Technion), Technion, Haifa, December 13-14, 1998
- (91) 1999: Invited talk
“Cytochrome P-450: Electronic Structure and Reactivity Patterns”
WATOC’99
August 1-6, 1999, Imperial College, London, UK
- (92-94) 1999: **Troisieme-Cycle Lecturer**
A series of 3 Lectures as a
VB paradigms, TSR, ET, Benzene Story
Basel, Sept. 1999
- (95) 1999: Invited talk
ESOC 11
“TSR Mechanism of Alkane Hydroxylation by Cytochrome P450”
July 23-28, 1999 Goteborg, Sweden
- (96) 1999: Invited talk
“TSR Mechanism of Alkane Hydroxylation and Olefin Epoxidation by
Cytochrome P450”
The First French-Israeli Meeting on Catalysis
December 19-23, 1999 , Paris, France
- (97) 2000: Invited talk
“Can Radicals be Both present and Absent? Alkane Hydroxylation by
Cyochrome P450”
The Israel Chemical Society Meeting
February, 2000, Beer-Sheva
- (98) 2000: Invited talk
“Cytochrome- Electronic Structure and Reactivity Trends in Hydrocarbon
Oxidation”
ICPOC 15
July 8-13, Goteborg, Sweden
- (99) 2000: Invited talk
“Hydroxylation by Cytochrome P450: Can radicals Be Both Present and
Absent?”
ICPP-1 Meeting
June 25-30, 2000, Dijon, France

- (100) 2000: Plenary Lecture
“Solving Puzzles in the Reactivity patterns of Cytochrome P450 Enzyme in Alkane Hydroxylation by Quantum Chemical Calculations”
Theoretical Chemistry Meeting: Electronic Structure: Predictions and Applications”
San-Sebastian, Spain, October 4-6, 2000
- (101) 2001: Plenary lecture (**The ICS Prize Talk**)
“An Excursion Into Valence Bond Theory”
The Israel Chemical Society Meeting
February 5-6, 2001, David Continental Hotel, Tel Aviv
- (102-104) 2001: Invited Series of Talks
A series of 3 Lectures as a
VB paradigms, Benzene Story, and P450 reactivity
Ecole Normale Superiure, May, 2001.
- (105-106) 2001: Two Talks (**The Kolthoff Prize Talks**)
“Iconoclasm or paradigm Shifts? A different Story of Benzene”
“Is there Anything New in Bonding? New Bonding Pardigms fromValence Bond Theory”
Department of Chemistry, The Technion, June 3-7, 2001
- (107) 2001: Plenary Lecture
“Entangled Mechanisms of Electron Transfer and Substitution of Ion Radicals- One Transition State Serves Two Different Mechanims”
ESOR VIII, Dubrovnik, Sept 1-6, 2001.
- (108) 2001: Invited Lecture
“Compound I of P450 and Its Analogs: Chameleon States”
The 12th Symposium on P450
La Grande Motte, France, Sept 11-16, 2001.
- (109) 2001: Plenary Lecture
“Mechanisms by which the Enzyme Cytochrome P450 Oxidizes Organic Compounds: How Can Radicals be Both Present and Absent?”
“Frontiers of Theoretical Chemistry”
Okazaki, Japan, Decemebr 17-19, 2001
- (110) 2002: Invited Lecture
“Mechanisms by which the Enzyme Cytocrome P450 Oxidizes Organic Compounds”
ADHOC 8
Atlanta, USA, June 2-7, 2002
- (111) 2002: Plenary Lecture
“Two-State Reactivity of Heme Protein Enzymes in Bond Activation”
Gordon Conference on Organo-Metallic Chemistry
Salve Regina University, USA, July 21-217, 2002
- (112) 2002 Plenary Lecture

“Mechanisms by which the Enzyme Cytochrome P450 Oxidizes Organic Compounds”.
The Second International Conference on Reactive Intermediates.
Ascona, Switzerland, July 17-12, 2002

- (113) 2002: Invited Lecture
“Two-State Reactivity of Heme Protein Enzymes in Mono-oxygenation”.
The Second Quantum Bioinorganic Chemistry (QBIC/2)
Orneas Castle, Sweden, July 29-31, 2002.
- (114) 2002: Invited Lecture
“Why Do Cytochrome P450 and Similar Hemoprotein Enzymes Need a Thiolate Ligand?”
The 66th Israel Chemical Society Meeting
Jerusalem, January 29-31, 2002
- (115) 2002: Plenary Lecture
“Entangled Mechanisms of Electron Transfer and Substitution Reactions of Ion Radicals – One Transition State Serves Two Different Mechanisms”.
The Workshop on Ultrafast Processes.
Algarve, Portugal, June 12-16, 2002.
- (116-118) Workshop, 5 hours on VB Theory
“New Bonding Paradigms from Valence Bond Theory”
“Valence Bond Diagrams: An Organizing Tool for Understanding Chemical Reactivity”.
The Minerva School
Blankensee, Germany, September 24-29, 2002.
- (119) 2002: Invited Lecture
“The protein, The Active Species and The Chameleon- A Story of P450”
The 1st THEOCHEM Meeting of the Israeli Theoretical Chemists
Jerusalem, October 9-10, 2002.
- (120) 2003: Plenary Lecture
“The protein, The Active Species and The Chameleon- Oxygen Transfer Reactivity Patterns of the Enzyme Cytochrome P450”
The Gordon Conference on Inorganic Reaction Mechanisms
Ventura, Ca., February 21-26, 2003.
- (121) 2003: Plenary Lecture
“The protein, The Active Species and The Chameleon- Oxygen Transfer Reactivity Patterns of the Enzyme Cytochrome P450”.
The Workshop on Ultrafast Processes.
Algarve, Portugal, June 12-16, 2003.
- (122) 2003: Plenary Lecture
“The protein, The Active Species and The Chameleon- Oxygen Transfer Reactivity Patterns of the Enzyme Cytochrome P450”.
13th International Conference on Cytochromes P450
Prague, Czech Republic, June 29-July 03, 2003
- (123) 2003: Plenary Lecture
“The protein, The Active Species and The Chameleon- Oxygen Transfer

Reactivity Patterns of the Enzyme Cytochrome P450".
 Computational Modeling of Catalysis
 Symposium at the Max-Planck-Institut für Kohlenforschung
 Mülheim, Germany, July 16-18, 2003

- (124) 2003: Invited Lecture
 "Reactivity Patterns of the Enzyme Cytochrome P450: The protein, The Active Species and The Chameleon".
 Making and Breaking Chemical Bonds in the Gas and Condense Phases: Theory and Applicatipons.
 226 ACS Meeting
 New-York City, USA, September 7-11, 2003
- (125-127) 2003: **3 Plenary Lectures**
 "The Protein, The Active Species and The Chameleon- Oxygen Transfer Reactivity Patterns of the Enzyme Cytochrome P450".
 "Multistate Reactivity of Compound I Reagents"
 "Two-State Reactivity (TSR); From Tiny Iron Oxo to Cytochrome P450..."
 Taiwan Bioinorganic Chemistry Symposium and Presymposium
 Hsinchu, Taichung, Taiwan, September 28-october 4, 2003.
 In addition: Lectures in the Technical University of Hong-Kong and In Xiamen University in China.
- (128) 2003: Invited Lecture
 "Oxidative reactivty of Cytochrome P450: The protein, The Active Species and The Chameleon"
 6th International Symposium on Electron Transfer
 Walberberg, Germany, October 29-November 1, 2003.
- (129) 2004: Plenary Lecture
 "Reactivity Patterns of Cytochrome P450"
 DFG Priority Program: Radicals in Enzymatic Catalysis
 Schloss Rauischholzhausen, Germany, February 18-21, 2004
- (130-131) 2004: Opponent
 "Ph.D Thesis of A. Bassan (student of P. Siegbahn) on Non-Heme Enzymes"
 Stockholm, May 5-8, 2004

 Gave also a Seminar on "Multistate Reactivity"
- (132) Plenary Lecture
 "Reacticity Patterns of Cytochrome P450 Enzymes"
 The Wolf Symposium Honoring H.B. Gray
 The Weizmann Institute of Sciences,
 Rehovot, Israel, May 11, 2004
- (133) Plenary Lecture
 "New Bonding Paradigms from Valence Bond Theory"
 The Symposium Honoring J. P. Malrieu
 Lagrasse, France, May 18-23, 2004
- (134) Plenary Lecture
 "Oxidative Reactivity Patterns of the Enzyme Cytochrome P450: the Protein, the Active Species and the Chameleon"

COFEM 2004, The Modena Fest
Venice, June 23-26, 2004

- (135, 136) **The Kurt Alder Lecture**
“One Reagent, Many Pathways: Two-State and Multi-State Reactivity Patterns-Bond Activation Reactions by Metal-Oxo Reagents”
Cologne, Germany, June 28, 2004
- Gave also a departmental Seminar: “Reactivity Patterns of the Enzyme Cytochrome P450: the Protein, the Active Species and the Chameleon”.
- (137,138) Two Invited Lectures in the Department of Chemistry, The University of Essen
“Oxidative Reactivity Patterns of the Enzyme Cytochrome P450: the Protein, the Active Species and the Chameleon”.
“One Reagent, Many Pathways: Two-State and Multi-State Reactivity Patterns-Bond Activation Reactions by Metal-Oxo Reagents”
Essen, Germany, July 13-16, 2004
- (139,140) A Planary Lecture, and A Roundtable Discutant
“New Bonding Paradigms from Valence Bond Theory”
EuroConference on New Theoretical and Spectroscopical Approaches to Inorganic Chemistry Problems
San Feliu de Guixoles, Spain, September 4-9, 2004
- (150) A Special Seminar Organized by Students
“New Bonding Paradigms from Valence Bond Theory”
The University of Barcelona, Spain, September 10, 2004
- (151-153) **A Lecture at a Special Student Seminar** (*Lecturers are voted by the students*)
“New Bonding Paradigms from Valence Bond Theory”
Department of Chemistry, the University of Minnesota
Minnesota, USA, October 20-24, 2004
- Gave also two more talks on P450
- (154) An Invited Lecture
“ One Reagent Many Pathways: Reactivity Patterns of Cytochrome P450 Enzymes and Analogous Catalysts”.
WATOC05
Captetwon, South Africa, January 15-21, 2005
- (155) **The Charles Coulson Lecture**
“What is New in Bonding: New Bonding paradigms from Valence Bond Theory”.
The University of Georgia, Athens, April 26, 2005
- (156) The Siegbahn Fest
“Reactivity Patterns of Cytochrome P450 Enzymes and Analogous Catalysts”.
Stockholm, Sweden, June 18-21, 2005.
- (157,158) The Gordon Conference on Drug Metabolism
“Reactivity Patterns of Cytochrome P450 Enzymes”.
Holderness College, New Hampshire, USA, July, 10-15, 2005.
Gave also a talk (on TSR) in the University of Rochester.

- (159-166) **An Invited Lecture Tour- India** (A series of 8 lectures in India (IIT Mumbai, TIFR Mumbai, IIS Bangalore, Ranbaxy Research Laboratories Delhi [2 talks], IICT Hyderabad, CLRI Chennai, CSIR Trivandrum).
The Protein, The Active Species and The Chameleon: Reactivity Patterns of Cytochromes P450”
“Two-State Reactivity: A General Reactivity Paradigm, From Iron Oxo Diatomic to P450 and Other Heme Protein Enzymes”.
“Structure and Reactivity of P450 Enzymes”.
India, September 29-October 20, 2005.
- (167) Malta II
“Research and Education in the Middle East”.
Invited to participate (one of 8 Israeli Scientists)
Malta, Nov 5-10, 2005.
- (168) A Plenary Lecture
“Theoretical Studies on P450 Mechanisms”
A Symposium Sponsored by the RSC and the Novartis Foundation,
London, Nov 15-16, 2005.
- (169-171) An Invited Lecture
“QM and QM/MM Studies of Enzymes and Large Molecules: Lessons and Specific Applications.”
The Satellite Symposium on Large Molecular Systems (Part of the XII International Congress of Quantum Chemistry).
Okazaki, Japan, May 17-19, 2006.
Gave two Invited Seminar in The University of Fukuoka and Nagoya.
- (172) Invited Seminar
“New Bonding Paradigms from VB Theory
The Weizmann Institute of Science
May 2006
- (173,174) Invited Lectures (2)
“Multi-state Reactivity Patterns of Cytochrome P450 and Nonheme Oxidation Catalysts” (Division of Inorganic Chemistry, Radical Metal Complex Chemistry).
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and Other Oxidation Catalysts” (Division of Inorganic Chemistry, Theoretical Inorganic Chemistry).
232nd ACS National Meeting, San Francisco, CA., September 10-14, 2006.
- (175) Invited Colloquium
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and Other Oxidation Catalysts”.
Department of Chemistry, the University of Aachen, Germany.
- (176,177) **The Christmas Lecture**
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and Other Oxidation Catalysts”.
Department of Chemistry, the University of Heidelberg, Germany.
(Gave a talk also in the Max Planck Institute in Mulheim).
December 11, 2006.

- (178) **The IQCB Lectureship** of the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences in Prague.
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and Other Oxidation Catalysts”.
May 21, 2007.
- (179) The 8th International ISSX Meeting
Sendai, Japan
“Quantum Mechanical Studies of P450 Catalyzed Reactions”.
October 9-12, 2007.
- (180) An invited Lecture
A Mini Symposium on Heme Enzymes
Tohoku University, Institute of Multidisciplinary research of Advanced Materials
“Can We Predict the Selectivity of P450 Enzymes?”
October 11, 2007.
- (181) An Invited Mini-course on VB Theory (12 Hours)
“Valence Bond Theory: Chemical Reactivity and the Nature of the Chemical Bond”
The Royal Institute of Technology, Department of Theoretical Chemistry.
Stockholm, Sweden
October 21-30, 2007.
- (182) A Plenary Lecture
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and other Oxidation Catalysts”.
The 9th FIGIPAS Meeting in Inorganic Chemistry
July 4-7, 2007, Vienna, Austria.
- (183) Malta III
“Research and Education in the Middle East”.
Invited to participate (one of 8 Israeli Scientists)
Istanbul, December 8-13, 2007.
- (184) A Plenary Lecture
The Milstein Fest
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and other Oxidation Catalysts”.
The Weizmann Institute, Rehovot, Israel
December 2, 2007.
- (185) A Plenary Lecture to the Public
“Chemistry: A Central Pillar of Human Culture”
“Madua’a”: The Hebrew University Series of Public Lectures
January 13, 2008.
- (186) A Kenote Lecture
“Can We Predict Enzymatic Selectivity: A Story of Cytochrome P450 Enzymes”.
The 73rd Annual Israel Chemical Society Meeting
Jerusalem, Israel
February 4-6, 2008.
- (187) A Plenary Lecture
“Two-State Rectivity – A General Reactivity Paradigm”.

The Dioxygen Activation Symposium: Global COE in Chemistry – Nagoya Special Symposium.
Nagoya, Japan
March 20-21, 2008.

- (188) A Plenary Lecture
“Can We Predict Enzymatic Selectivity?”
International Symposium on Advance Science and Biotechnology 2008.
Osaka, Japan
March 22-23, 2008.
- (189) A Plenary Lecture
“Bonding in Oxymyoglobin: Is it Pauling, Weiss, McClusre-Goddard? None? All?”
Theoretical Biochemistry – Methods and Applications.
Stockholm, Sweden
May 14-17, 2008.
- (190) A Plenary Lecture
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and other Oxidation Catalysts”
The 38th ICC International Congress
Jerusalem, July 20-24, 2008.
- (191) An Invited Lecture
“A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and other Oxidation Catalysts”
Department of Chemistry, Ewha Women University
Seoul, Korea, September 9-12, 2008.
- (192) **The Schrödinger Medal Lecture**
“Concepts and Applications in Chemical Reactivity”
WATOC08 International Congress
Sydney, Australia, September 14-19, 2008.
- (193) An Opponent in the PhD Examination of Dr P. Schyman, and an Invited talk
“Reactivity Patterns of the Enzyme Cytochrome P450: What A Versatile Catalyst It Is!”
Stockholm University
Stockholm, October 29-31, 2008.
- (194) An Invited Lecture
“Two and Multi State Reactivity: From Iron Oxo Diatomic to Cytochrome P450 and Nonheme Synthetic Complexes”
Gas Phase Ion Chemistry: State of the Art and Perspectives.
An International Symposium (in Honor of H. Schwarz)
Eberbach, Germany, December 14-16, 2008.
- (195) Plenary Lecture
“What Did We Learn from Theory about Structure and Reactivity Patterns of the Enzyme Cytochrome P450?”
The Gordon Conference on Metals in Biology
Ventura, Ca., January 25-30, 2009.
- (196) Plenary Lecture

“Cytochrome P450: What A Wonderful Catalyst It Is?”
The School of Pharmacy, The Hebrew University
Hadassa Medical School, February, 5, 2009.

- (197) Plenary Lecture
“Cytochrome P450: What A Wonderful Catalyst It Is?”
Final Symposium of the Sonderforschungsbereich 424
Munster, Germany, February 12-14, 2009.
- (198) Plenary Lecture
“Cytochrome P450: What A Wonderful Catalyst It Is?”
The Schulich International Symposium Series
Technion, Haifa, March 1, 2009.
- (199) Plenary Lecture
“Cytochrome P450: What A Wonderful Catalyst It Is?”
The 25th Anniversary of Theoretical Chemistry Network of Catalonia, and the 65th
Birthday Fest of S. Olivella. Symposium on “Theoretical Chemistry: Modeling
reactivity from Gas Phase to Biomolecules and Solids”
Barcelona, June 29- July 3rd, 2009.
- (200) Keynote Lecture
“Cytochrome P450: What A Wonderful Catalyst It Is!”
The 42nd IUPAC Congress
Glasgow, August 3-7, 2009
- (201) Invited Lecturer
“Valence Bond Modeling and Density Functional Theory Calculations of
Reactivity and Mechanism of Cytochrome P450 Enzymes: Thioether
Sulfoxidation”
The 145 Faraday Discussion: “Frontiers of Physical Organic Chemistry”
Cardiff, September 2-4, 2009
- (202) Invited Lecture
“Cytochrome P450: What A Wonderful Catalyst It Is!”
The Mini-symposium of the WCU Group
Ewha Womens University
Seoul, Korea, November 16, 2009
- (203) Plenary Lecture
The Schulich Mini-symposium on ‘Frontiers in Computational Chemistry, Bridging
Chemistry and Biology’
“Two-State Reactivity All the Way: From Iron-Oxo Diatomic To Cytochrome P450
and Other Bond Activating Catalysts”
The Technion
Haifa, Israel, December 08, 2009
- (204) Invited Lecture
“Is There Anything New in Two-Electron Bonding? Charge-Shift Bonding”
High School Teachers Workshop – The Weizmann Institute
January 6, 2010
- (205) Plenary Lecture
The Thiel-Fest Symposium,

“Is There Anything New in Two-Electron Bonding? Charge-Shift Bonding”
The Max Planck institute in Mülheim,
Mülheim, Germany, February 28-March 2, 2010.

- (206) The Chava Lifshitz Memorial Lecture,
“Is There Anything New in Two-Electron Bonding? Charge-Shift Bonding”
March 14, 2010.
- (207) Plenary Lecture – The Leonard N. Owen Lectureship
“Is There Anything New in Two-Electron Bonding? The Charge-Shift Bond”
Imperial College, London, June 4th, 2010.
- (208) Invited Talk
The Mini-symposium of the GRL Group
“Potential Theoretical Studies of O₂ evolution”
Ewha Womens University
Seoul, Korea, June 18, 2010
- (209-212) **Invited Lectureship Series: SCILS- Scientific Computing International Lecturer Series**
Talks on:
“What A Versatile Catalyst: Cytochrome P450 and Its Reactivity Patterns”
“Bonding in Oxy Myoglobin and Hemoglobin: Controversies, Surprizes and take Home Lessons”
A Public Talk – “Chemistry A Central Pillar of Human Culture”
The University of Cape Town, Cape Town South Africa, August 19-Sept 02, 2010
- (213) Invited Talk
Chemistry at Spin Centers International Symposium 2010
“Bond Activation Patterns by Oxo-Metal Reagents in Enzymes and Synthetic Models”
Bad Honnef, Germany, September 22-24, 2010.
- (214) A Talk in the SKLMRD & Theoretical Center Invited Talks Series
“What A Versatile Catalyst: Cytochrome P450 and Its Reactivity Patterns”
State Key laboratory of Molecular Reaction Dynamics, Dalian, China, September 29, 2010
- (215) Invited Lecture in The Seminar Series of Gratz
“What A Versatile Catalyst: Cytochrome P450 and Its Reactivity Patterns”
Gratz, Austria, October 15, 2010
- (216) Scientific Evaluator of the theory section
International Board Meeting of the State Key laboratory Institute
Xiamen, China, December 04-10, 2010

Gave a talk on P450
- (217) Invited Lecture
“Why Does Nature Use High-Spin Enzymes for Bond Activation?”
QBIC-3, Cesky Krumlov, Czech Republic, June 25-28, 2011
- (218) Invited Lecture

“Why Does Nature Use High-Spin Enzymes for Bond Activation: The Concept of Exchange-Enhanced Reactivity”
WATOC 011, Santiago de Compostella, Spain, July 14-23, 2011

- (219) Invited Lecture
“The Valence Bond Way in Bioinorganic Chemistry”
The Satellite Conference on Highly Correlated Methods,
A Corunia, Spain, July 24-25, 2011
- (220) Invited Lecture STC 2011
“Reactivity Patterns of Bond Activation by Metal Oxo Complexes”
The 47th Symposium of Theoretical Chemistry on ‘Designing Molecular
Functionality: Challenges for Theoretical Approaches’,
Sursee, Switzerland, August 21-25, 2011
- (221) Invited Lecture
“The Valence Bond Way in Bioinorganic Chemistry”
Conference on Challenges in Computational Homogeneous Catalysis
Stockholm, Sweden, August 25-27, 2011
- (222) Plenary Lecture (cancelled participation due to nuclear events in Japan)
ISTCP-VII, Tokyo, September 2-8, 2011
- (223) Plenary Lecture
“MOLMOD 2011: Modeling of Molecular Properties”
“Reactivity Patterns of Metal Oxo Reagents”
Heidelberg, October 8-11, 2011.
- (224) Plenary Lecture
“WISPOC 2012”
“The Valence Bond Way in Chemistry”
Bersanone, Italy, January 26 – February 3, 2012.
- (225) Plenary Lecture
“Sanibel 52”
“The Valence Bond Way in Chemistry”
St. Simon Island, Georgia, USA, February 19-25, 2012.
- (226) Colloquium
“Cytochrome P450: What a Wonderful Catalyst it Is!”
Department of Chemistry, University of Aachen, April 20, 2012
- (227-232) A series of 6 talks (50 min. each)
“Cytochrome P450: What a Wonderful Catalyst it Is!” (2 talks)
“New Paradigms in Bond-Activation Reactivity of Metal-Oxo Complexes” (2 talks).
“What’s New in Chemical Bonding? Charge Shift Bonds”
“What’s New in Chemical Bonding? No Pair Bonds and More”
The Max Plank Institute of Bioinorganic Chemistry, Mülheim, April 22-26th, 2012
- (233) Frontiers in Biological Chemistry Award Lecture
“Understanding Oxidative Reactivity: An Excursion fro H + H₂ to Cytochrome”.
The Max Plank Institute of Bioinorganic Chemistry, Mülheim, April 22-26th, 2012
- (234) Plenary Lecture

The Joint Israeli-French Meeting on Theoretical Chemistry
 “Reactivity Patterns of Metal Oxo Enzymes and Reagents”
 Israel Academy of Sciences and Humanities, Jerusalem, May 14-15, 2012

- (235) Plenary Lecture
 “The Valence Bond Way in Chemistry”
 ESPA2012
 Barcelona, June 28-30, 2012
- (236-237) Two Plenary Lectures (50 min. each)
 “The Valence Bond Way in Chemistry”
 The VB Workshop
 Paris, July 17-23, 2012
- (238) Invited Lecture
 EuChems4
 “The Valence Bond Way in Chemistry”
 Prague, August 26-30, 2012
- (239) Plenary Lecture
 ADHOC 2012
 “Reactivity Patterns of Metal Oxo Enzymes and Reagents”
 Ramat Rachel, Jerusalem, September 2-7, 2012.
- (240) Plenary Lecture
 The ICS 78th Annual Meeting
 “New Wines in Old Flasks”
 Tel Aviv, Dan Panorama Hotel, February 12-13, 2013.
- (241-2) Two Lectures
 Nanyang Technical University
 “Cytochrome P450: What a Wonderful Catalyst it Is!”
 “Why Does Nature Use High-Spin Enzymes for Bond Activation: The Concept of
 Exchange-Enhanced Reactivity”
 Singapore, February 24-March 3rd, 2013
- (243-246) Plenary Lecture
 Congresso Argentino XVIII
 “Exchange-Enhanced Reactivity: A Theory of Bioinorganic Reactions”
 Rosario, Argentina, April 9-12, 2013.
 Three Lectures (Seminar Tours), March 22-April 8, 2013
 Universities of Buenos Aires, Cordoba, and Rosario
 “What is New in Bonding? New Bonding Paradigms from Valence Bond Theory”.
- (247) **A Scrocco Colloquia Lectureship**
 Scuola Normale Superiore di Pisa, May 29, 2013.
 “Cytochrome P450: What a Wonderful Catalyst it is!”
- (248) Invited Talk
 ICBIC 16
 Grenoble, France, July 21-27, 2013
 “Reactivity Patterns of Metal Oxo Enzymes and Reagents”

- (249) **Plenary Lecture**
The R. Neumann 60 Birthday Fest Symposium
The Weizmann Institute, Rehovot, Israel, October 25th, 2013
“A New Theory of Bioinorganic Chemistry”.
- (250) **Plenary Lecture**
The Lise Meitner Beirat Symposium
The Weizmann Institute, Rehovot, Israel, November 4th, 2013
“Bonding with Parallel Spins”
- (251) **Plenary Lecture**
The S. Hoz Fest Symposium
Bar Ilan University, Ramat Gan, Israel, January 7th, 2014
“From the Hydrogen Exchange all The Way to Bond Activation by Cytochrome P450: The Valence Bond Way”
- (252) **The Lu Jiayi Lectureship Award** in The State Key Laboratory, University of Xiamen, Xiamen, China December 3, 2013).
“From the Hydrogen Exchange all The Way to Bond Activation by Cytochrome P450: The Valence Bond Way”
- (253) Invited Lecture
Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, 155 Yangqiao Road West, Fuzhou, 350002 ,P.R.China, December 7th, 2013.
“Cytochrome P450: What a Wonderful Catalyst it Is!”
- (254) Invited GDCh Lecture
The Institute of Chemistry, Münster University
Münster, Germany, April 14th 2014
“Exchange-Enhanced Reactivity- A New Theory of Bioinorganic Chemistry”
- (255) Invited GDCh Lecture
The Institute of Chemistry, The University of Giessen
Gissen Germany, April 15th, 2014
“New Wines in Old Flasks: What is New in Electron Pair Bonding?”
- (256) Invited GDCh/AvH/UniCat Lecture
The Institute of Chemistry, TU Berlin, Free University of Berlin, and The Humboldt University
Berlin, Germany, May 5th 2014
“Cytochrome P450: What a Wonderful Catalyst it Is!”
- (257) Invited Lecture
BASF Company
Mannheim, Germany, May 19th 2014
“From the Hydrogen Exchange all The Way to Cytochrome P450: The Valence Bond Way”
- (258) Invited Lecture
The University of Munich

Munich, Germany, May 19th 2014
 “From the Hydrogen Exchange all The Way to Cytochrome P450: The Valence Bond Way”

- (259-272) A Series of Lectures (12.5 hours in total)
 The Technical University of Berlin,
 Berlin, Germany, April 23rd –May 28th 2014
 “From H₂ and Allyl Radical to Reactivity of Cytochrome P450 Enzymes, and More... The Valence Bond Way”.
- (273) Invited Lecture
 iCHAT, Rome, June 22-26, 2014
 “Reactivity Patterns in H Transfers”.
- (274) Invited Lecture
 ICPOC 22, Ottawa, Canada, August 10-15, 2014
 “Reactivity Patterns of Metal Oxo Enzymes and Reagents”
- (275) Invited Lecture
 WATOC 2014, Santiago de Chile, October 5-10, 2014
 “New Aspects of Bonding and Reactivity”
- (276-7) Two Invited lectures
 Xiamen University, November 3 and 5, 2014
 “Chemistry – A Central Pillar of Human Culture” (a public talk)
 “Cytochrome P450: What a Wonderful Catalyst It is!” (a colloquium)
- (278) Invited Lecture
 The Z. Gross Fest Symposium
 The Technion, Haifa, Israel, February 19th, 2015
 “New Concepts for Chemical Reactivity”
- (279-282) A Series of Four Lectures
 University of Paris VI, April 1-15, 2015
 “New Wines in Old Flasks: Charge Shift Bonding in Chemistry”
 “Chemistry – A Central Pillar of Human Culture” (a public talk)
 “Cytochrome P450: What a Wonderful Catalyst It is!” (a colloquium)
 “Exchange Enhanced Reactivity: New Principles of Reactivity for Oxo-Complexes and Enzymes”.
- (283,284) **Two Lectures (Plenary and Keynote)**
 The Chemical Bond in the 21st Century
 Xiamen, China, June 14-18, 2015
 “Carbon Breaks the Glass Ceiling of Triple Bonding”.
 “The Computational Paradise: Use of VB Theory for Understanding Chemical Reactivity”
- (285) **Plenary Lecture**
 ESOR 2015, Kiel, Germany, August 30th-September 5th, 2015
 “Does Carbon Break the Glass Ceiling of Triple Bonding?”
- (286) Invited Lecture
 “Does Carbon Break the Glass Ceiling of Triple Bonding?”
 The Technical University of Berlin

Berlin, Germany, September 9, 2015.

- (287) Invited Lecture
“How to Understand Chemical Reactivity Using Valence Bond Ideas?”
A Seminar for Graduate Students
The University of Munich
Munich, Germany, September 21st, 2015
- (288) Invited Lecture
“Does Carbon Break the Glass Ceiling of Triple Bonding?”
The Free University of Berlin
Berlin, Germany, September 28, 2015.
- (289) Invited Lecture
“Reactivity Pattern of Metal Oxo Reagents and Enzymes”
The Max Planck Institute of Biophysics
Göttingen, Germany, Nov. 10, 2015.
- (290) Invited Lecture
“Why Does Nature Utilize High Spin Species to Activate C-H Bonds?”
The Inter-Academy Symposium:
Of the Israel Academy of Sciences and Humanities
And the German national Academy of Sciences, Leopoldina
Jerusalem, Nov. 9-10, 2015.
- (291) Invited Lecture
“Why Does Nature Use Enzymes with High-Spin States to Activate C-H Bonds?”
The Harry Gray 80th Birthday Symposium
The Schulich Winter School of Chemistry, The Technion
Haifa, December 1-3, 2015.
- (292) **Scientific Perspective Lecture**
“A Theory for Bioinorganic Chemical Reactions: Can Multireference and
Multiconfiguration Methods Contribute?”
Molcas2016: Molcas Developers’ Workshop 2016
Vienna, Austria, March 30- April 1, 2016.
- (293) Invited Lecture
“New Smart Reagents in Chemistry – Oriented Electric Fields”
The 70th Fujihara Seminar
Fukuoka, Japan, April 17-21, 2016
- (294) Invited Lecture
“Why Did Nature Select Metallo-Enzymes that Use High-Spin Reactive Species to
Activate Strong C-H Bonds?”
The Hebrew University – Bangalore Bioinstitutional Meeting
Jerusalem, Israel, April 12-13, 2016
- (295) Invited Lecture
“Why Did Nature Select Metallo-Enzymes that Use High-Spin Reactive Species to
Activate Strong C-H Bonds?”
The XVII Workshop CECAM: Structural and Functional Annotation of
Bioinorganic Systems: Perspectives and Challenges from Theory and Experiment
Scuola Normale Superiore, Pisa, Italy, May 23-26, 2016.

- (296) **VIP Lecture**
“On the Nature of the Halogen Bond!”
ISXB2: 2nd International Symposium on Halogen Bonding
Goteborg, Sweden, June 6-10, 2016.
- (297) Keynote Lecture
“Cytochrome P450: What a Wonderful Catalyst It Is!”
The 13th International Meeting on Cytochrome P450 Biodiversity and Biotechnology
Vancouver, Canada, July 22-26, 2016.
- (298) Invited Lecture
“Description of Research Achievements”
The Annual Meeting of the International Academy of Quantum Molecular Science (IAQMS)
Menton, France, July 1-4, 2016
- (299) Keynote Lecture
“Valence Bond - What a Wonderful Theory It Is!”
The Conference on: Advancing the Frontiers of Chemistry with Valence Bond Approaches
University of Uppsala, Uppsala, Sweden, June 23-25, 2016.
- (300) The Opening Lecture of the GDCh Series of 2016/2017
The Institute of Chemistry, TU Berlin, Free University of Berlin, and The Humboldt University
“New Smart Catalysts/Inhibitors in Chemistry – Oriented Electric Fields”
Berlin, Germany, October 24th 2016
- (301-302) Keynote Lectures
“The Lise Meitner Center – What a Marvelous Achievement It Was!”
“One’s Personal Account on Science During the Membership in the Lise Meitner Center”
The Golden Symposium of The Lise Meitner Center
Jerusalem, February, 11-12, 2017
- (303) Keynote Lecture
“New Smart Reagents in Chemistry – Oriented Electric Fields”
The Symposium on Electron Localization and Delocalization: Theory, Measures and Applications in Chemistry.
The 100th Canadian Chemical Society (CSC) Meeting
Tonoto, Canada, May 28 – June 1st, 2017.
- (304) Keynote Lecture
2nd International Conference of Hydrogen Atom Transfer (iCHAT)
“Reactivity Patterns: Reactivity, Selectivity and Spin-State Selectivity”
Frascaty, Italy, July 2-7, 2017.
- (305) Keynote Lecture
“Oriented Electric Fields As Future Reagents in Chemistry Fields”
The 254 ACS Meeting (The Roald Hoffmann 80th Birthday Symposium)
Washington DC, August 20-25th, 2017
- (306) Keynote Lecture

“Oriented Electric Fields As Future Reagents in Chemistry Fields”
 The Triennial Congress of the World Association of Theoretical and Computational Chemists, WATOC 2017
 Munich, Germany, August 27 - September 1, 2017.

- (307-308) Plenary Lectures
 The Chemical Bond at the 21st Century – 2017
 “The Landscape of Chemical Bonding: Some New Features Emerging from Valence Bond Theory”
 “The Valence Bond Way: Reactivity Modeling”
 Conference and Tutorials
 Aachen, Germany, September 2-7, 2017
- (309-311) **Invited Series of Lectures**
 “Oriented Electric Fields – New Effectors in Chemistry”
 The University of Groningen – **The Stratingh Lectureship**
 The university of Utrecht
 The Free University of Amsterdam
 The Netherlands, May 21-26, 2018
- (312) **Plenary Lecture**
 NOSIC 8
 “Chemistry – A Central Pillar of Human Culture”
 Prullans de Cerdanya, Spain, June 6-10, 2018.
- (313) Invited Lecture
 16-ICQC Meeting
 “Oriented Electric Fields – New Effectors in Chemistry”
 Menton, June 16-24, 2018.
- (313) Invited Lecture
 VALBO-1, “Understanding Chemistry and Biochemistry Using Conceptual Models”
 “Oriented Electric Fields – New Effectors in Chemistry”
 Marseilles, France, June 25-28, 2018.
- (314) **Plenary Lecture**
 VALBO-1 Tutorial Sessions, “Understanding Chemistry and Biochemistry Using Conceptual Models”.
 “Valence Bond Diagrams: A Unified Paradigm for Understanding Chemical Reactivity”
 Marseilles, France, June 25-28, 2018.
- (315) Keynote Lecture
 International Symposium of Reactive Intermediates and Unusual Molecules (ISRIUM 2018)
 “Oriented Electric Fields – New Effectors in Chemistry”
 Ascona (Monte Verità), Switzerland, July 15-20, 2018.
- (316) Invited Seminar
 The Institute of Chemistry, TU Berlin (Theoretical Chemistry and Gas-phase Chemistry Groups)

“Kinetic isotope effect: A sample of the Reactive Spin-State and the Stereo Chemistry of the Transition State During Hydrogen Abstraction Reactions of Oxoiron (IV) Complexes and Enzymes”.
September 5th, 2018, Berlin, Germany

- (317) **Plenary Lecture**
ISRANALYTICA – The 22nd Annual Meeting of the Israel Analytical Chemistry Society
“The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music”
January 22-23, 2019, David Intercontinental Hotel, Tel Aviv, Israel
- (318) **Plenary Lecture: The Platinum Jubilee Lecture**
CSIR – Indian Institute of Chemical Technology (IICT) Hyderabad
The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music”
February 11, 2019, Hyderabad, India
- (319) **Plenary Lecture**
NIICT Trivandrum
The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music”
February 15, 2019, Trivandrum, India
- (320) **Plenary Lecture**
IISC Bangalore
“Oriented Electric Fields – New Effectors in Chemistry”
February 17, 2019, Bangalore, India
- (321) **Honorary Plenary Lecturer**
International Conference on Advanced Chemical and Structural Biology (ICACSB) 2019
“Oriented Electric Fields – New Effectors in Chemistry”
February 19-21, 2019, Chennai, India
- (322) **Plenary Lecture**
The Chemical Engineering Association of the AEAI (Association of Engineers and Architects in Israel)
Celebration of the “Corner Stone” of the Profession
The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music” [Given in Hebrew].
March 5, 2019, 200 Dizengoff St., Tel Aviv, Israel
- (323) **Plenary Lecture**
The Israel Academy of Sciences
The Symposium Marking “100 Years Since the Birth of Primo Levi and 150 Years to the Publication of the Periodic Table by Mendeleev”,
The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music” [Given in Hebrew].
May 6, 2019, The Academy Building, Jerusalem.
- (324) **Invited Lecture**

The Wenner-Gren Foundation International Symposium, “Mechanistic Homogeneous Catalysis. A Meeting Between Theory and Experiment”
“Oriented Electric Fields – New Effectors in Chemistry”
September 4-6, 2019, Stockholm (the Wenner-Gren Building), Sweden

- (325) **Plenary Lecture**
European Symposium on Organic Reactivity (ESOR) 2019.
“Oriented Electric Fields– New Effectors in Chemistry”
September 8-13, 2019, Dubrovnik, Croatia.
- (326) **The Opening GDCh Colloquium**
The Technical University of Berlin
“The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music”
September 23, 2019
- (327) **The Solvay Colloquium**
The Solvay Institute, Brussels, Belgium
“Oriented Electric Fields– New Effectors in Chemistry”
October 1, 2019, Free University of Brussels, Brussels, Belgium
- (328) **The Opening Colloquium of the 2019/2020 Academic Year**
The Hebrew University of Jerusalem
“The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music”
October 30, 2019, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel
- (329) **Invited Lecture**
Israel-Japan Conference on “Molecular Catalysis in the Service of Society”
“Oriented Electric Fields– New Effectors in Chemistry”
November 3-5, 2019, The Schulich Faculty of Chemistry, Technion, Israel Institute of Technology
Haifa, Israel.
- (330) **Invited Lecture**
The Teacher-Researcher Program Symposium on “Introduction of Natural Sciences”
“The Periodic Table – A Universal Icon: Its Birth 150 Years Ago, and Its Popularization through Literature, Art and Music” [Given in Hebrew].
24/11-31/12 2019, The Hebrew University, Jerusalem.
- (331) **Invited Lecture**
The 85th, Israel Chemical Society Meeting
“Oriented Electric Fields– New Effectors in Chemistry”
February 18-19, 2020
Jerusalem Congress Center, Israel
- (332) **The Van’t Hof Lecture**
The PAC Symposium
“Oriented Electric Fields– New Effectors in Chemistry”
Leiden, March 5, 2020
- (333) **A Zoom Invited Talk**

The SFB Program in the Three Universities of Berlin
 "A New Family of Bonds - Charge-Shift Bonding"
 Berlin, February 15, 2021.

6. RESEARCH GRANTS

- 1979-1981: Israel Ministry of Absorption IL. 250,000 for
 "Construction of Potential Energy Surfaces"
- 1981-1983: Israel Academy of Sciences IS 125,000/year for
 "Non-bonded Interactions in Organic Chalcogen Compounds"
 In collaboration with J. Bernstein and A. Ullman.
- 1982-1983: Rector's Discretionary Fund, \$8,000 for
 "Design, Synthesis and Characterization of Novel Organic metals"
 In collaboration with the members of the Organic Metals Group at BGU.
- 1983-1986: Israel Academy of Science \$20,000 for
 "Design, Synthesis and Characterization of Novel Organic Metals"
 In collaboration with the Organic Metals Group at BGU.
- 1983-1985: Wolf Foundation \$27,000 for
 "Organic Metals"
 In collaboration with the Organic Metals Group at BGU.
- 1985-1988: Haselblad Foundation \$40,000 for
 "Organic Metals"
 In collaboration with the Organic Metals Group at BGU.
- 1987-1990: Israel Council for Research and Development - BMFT DM 318,000
 for "Organic Conductors"
 In collaboration with the Organic Metals Group at BGU.
- 1987-1990: United States Army European Office of Research, \$119,700 for
 "Electrically Conducting Materials: Design, Synthesis and
 Characterization".
 In collaboration with the Organic Metals Group at BGU.
- 1989-1991: Israel Academy of Sciences \$22,500/year for
 "A Search for Significance in Reactions between Electrophiles and
 Nucleophiles".
- 1990-1991: Rector's Discretionary Fund, \$15,000 for
 "Theoretical Studies of Chemical Reactivity".
- 1992-1993: The Hebrew University's Discretionary Funds, \$140,000
 A Startup fund to acquire and upgrade computer facilities for carrying out:
 "Computational Quantum Chemical Studies"
- 1992-1993: The Hebrew University Discretionary Fund, \$24,000 for
 "What Structural and Bonding Patterns are Possessed by Transition
 States of Organic Electron Transfer Reactions in Comparison with their
 Bond Forming Analogs?"

- 1992-1995: Israel Academy of Sciences, \$144,000
for "What Structural and Bonding Patterns are Possessed by Transition States of Organic Electron Transfer Reactions in Comparison with their Bond Forming Analogs ?"
- 1993: The Ministry of Science and Technology (MOST), IS 37,500 for
"Transition State Paradigms in Organic Chemistry".
- 1994: The Hebrew University Discretionary Fund, \$10,000 for
"Reactivity and Structure in Large Many Electron Systems".
- 1994-6: The Volkswagen Foundation, DM 54,000 for
"Electron transfer in Organic and Transition Metal Gas-phase Ion Chemistry" (with H. Schwarz and D. Schröder).
- 1995: Vatat, The Israeli Committee For Financing and Budgeting Science,
\$ 260,000 for purchasing computing facilities to carry out quantum chemical calculations.
- 1997-present: MINERVA:
DM 4,000,000 endowment fund, and DM 1,150,000 for equipment:
To Establish A Center of Computational Quantum Chemistry (with Y. Apeloig, The Technion).
- 1996-1999: Israel Science Foundation
"Bonding Patterns in Ground and Excited States"
\$ 42,000/y for three years
- 1997-1999: The German Israeli Foundation
"Spin Inversion Mechanisms in Chemical Reactions: Selectivity Patterns." (with S. D. Peyerimhoff)
DM 80,000-90,000/y for three years
- 1997-2001: The Volkswagen Foundation
"Electron transfer in Organic and Transition Metal Gas-phase Ion Chemistry" (with H. Schwarz and D. Schröder).
DM 115,000 for three years
- 1999-2002: ISF,
"A Computational Quantum Chemical Study of Hydrocarbon Oxidation by Cytochrome P450 and Model Transition Metal Complexes"
\$ 40,000/y for three years
- 2000-2003: Ministry of Science and Technology
"Catalytic Oxygen Transfer and Oxahalogenation: From Biomimetic Systems to Industrial Catalytic Processes"
IS 200,000/y for three years
- 2001-2002: Niedersachsen Foundation
"Anti-Tumor Pharmacophors (Endiyne and Enyne-Allene Chemistries) and Their Reactivity Control: Interplay of Theoretical Analyses and Experimental Investigations"
DM 25,000/y for two years.

- 2000-2001: The European Commission, Marie Curie Individual Fellowships
“A Theoretical Study of hydrocarbon oxidation by Cytochrome P450 and Model Transition Metal Complexes”.
EURO 132,000 for two years.
- 2000-2001: Robert Szold Foundation
“Development and Implementation of s Density Functional Software for Computation of Large Molecules with Open Electronic Shells”.
\$24,000 for one year
- 2001-2004: The German Israeli Foundation
“A Computational Study of Species in Catalytic Cycles of Mono-Oxygenase and Peroxidase Enzymes in their Protein Environment by Combined Quantum Mechanical/Molecular Mechanical Methods”.
€ 30,000/y for three years
- 2002-2005: The Israeli Science Foundation
“Chameleon and Multi-State Oxidants: Studies of Structural and Reactivity Trends of Active Species of Heme-Protein Enzymes by Computational Quantum Chemical methods”
\$46,000/y for four years.
- 2003-2005: The Franco-Israeli Research Grant
“Interplay of Experimental and Theoretical Studies of C-X Bond Activation by Anionic Complexes of Pd(0): What makes for a Good Catalytic Cycle?”
\$30,000/y for two years.
- 2005-2009: DIP (Deutsche – Isralische–Project), BMBF
Functionalization of Unreactive Molecules
€ 50,000/y for five years.
Computing Equipment: € 40,000/y 1st year, USD 10,000 2nd year.
- 2006-2009: The Israeli Science Foundation
“Studies of Structure-Function Relationships in Peroxidase and Heme Oxygenase Enzymes by Means of Computational Quantum Chemistry”
\$44,000/y for three years.
\$ 30,000 for computing equipment.
- 2009-2013: The Korean Government
“Bioinspired Chemistry”
A 5 Years Grant within the World Class University (WCU) Project (with W. Nam, J. Valentine, K. Karlin, S. Fukuzumi)
Won 300,000,000/y
- 2009-2010: The Minerva Foundation
An Equipment Grant to the Lise Meitner Center
EUR 38,000.
- 2009-2013: The Israeli Science Foundation
“Quantum Chemical Investigations of Brain Chemistry Mediated by Heme and Nonheme Enzymes”
52,000 USD/y

- 2010-2011: The University of Michigan Outsourcing Grant
“QM/MM Investigation of P450 2B4”
45,000 USD.
- 2011-2015: The NIH
“Microsomal Cytochromes P450 and their Interactions with their Redox Partners”
63,000 USD/y for four years
- 2011-2012: The Minerva Foundation
Special Grant on Molecular Catalysis
EUR 50,000.
- 2012: The Minerva Foundation
Special Grant on Intermolecular Interactions
EUR 60,000.
- 2013-2014: The Minerva Foundation
An Equipment Grant to the Lise Meitner Center
EUR 50,000.
- 2013-2017: The Israeli Science Foundation [1183/13]
“Quantum Chemical Investigations of Reactivity Patterns of Nonheme Enzymes”
65,000 USD/y for 4 years.
- 1997-2017: The Minerva Foundation
A Yearly Grant for the Lise Meitner Center
Approximately 150,000 USD/y
- 2018-2022: The Israeli Science Foundation [520/18].
“Electric Fields as New Effectors of Selective Chemical Changes”
250,000 IS/y for 4 years.

7. AWARDS, HONORS

- 1973: The Israel Chemical Society Award for B.Sc. students.
- 1973: The Bar-Ilan University Award for M.Sc. students
- 1974-9: Israel - United-States Educational Foundation, Fulbright Fellow.
- 1980: Deutscher Akademischer Austauschdienst, DAAD Fellow.
- 1984-5: CNRS (France), "Poste Rouge".
- 1985: NSERC (Research Council of Canada), International Exchange Award.
- 1985: Rothschild Foundation (Geneva), Fellowship for writing a monograph.
- 1988: The 1988 Israel Chemical Society Medal Award for the Outstanding Young Chemist.

- 1995: Lise Meitner-Alexander von Humboldt Senior Research Award.
- 1995: The E. D. Bergmann Prize, Given by The Academy of Sciences and Humanities in Israel.
- 1997: Included in the ISI list of "The 1000 Most Cited Chemists in the Years 1981-1997".
- 2001: The Israel Chemical Society Excellence Award for the year 2000 (*"for his seminal work in chemical reactivity and bonding"*).
- 2001: The Kolthoff Prize for the year 2000/2001 (*"for his seminal contribution to the understanding of the chemical bond, reaction mechanisms and electron transfer processes in organic chemistry"*), The Technion, Israel.
- 2002: Elected as member of the Scientific Board of WATOC.
- 2003: Elected Fellow of the (AAAS) (American Association for the Advancement of Science); (*"for distinguished contributions to the field of valence bond theory, contributing new ideas and thought-provoking models that have helped to rechart the mental map of chemistry"*).
- 2004: Selected, by the University of Köln, as **the Kurt-Alder Lecturer** (for *"ground-breaking in theoretical and computational chemistry, aiming at the understanding of chemical and biochemical reactivity, in particular with respect to the revolutionary concept of multistate reactivity in organometallic chemistry and catalysis"*).
- 2004 (Fall) The University of Minnesota Lectureship (selected by the graduate students committee).
- 2005: Selected by the University of Georgia, Athens, as **The Charles Coulson Lecturer**.
- 2006: Selected by the University of Heidelberg, Germany, as The Christmas Lecturer of the Graduate School of Chemistry.
- 2007: Selected by the Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences in Prague as **the IOCB Lecturer** for May 2007.
- 2007: The Schrödinger Medal for the outstanding computational chemist for 2007 (The medal is awarded to S. Shaik for *"his outstanding contributions to the understanding of the chemical bond, reaction mechanisms in organic chemistry, and enzymatic reactivity"*).
- 2007: As a recipient of the Schrödinger Medal, I became also a WATOC Fellow.
- 2008: **The Schrödinger Medal Lecture Award**
WATOC 2008, Sydney Australia
- 2010 (June): Selected as **the Leonard N. Owen Lecturer** at the Imperial College –London.
- 2010 (August) Selected as the **1st Lecturer for the International Lectureship Series** for Computational Science: SCILS- The University of Cape Town.

- 2007-2011: Appeared in the list of Chemists with the H index higher than 50. Published in: www.rsc.org/chemistryworld/News/2007/April/23040701.asp
Updated on April 15, 2010.
- 2012 (Spring) Awarded, by the board of directors of the Max Planck Institute in Mülheim, with the “**Frontiers in Bioinorganic Chemistry Lectureship**”.
- 2102 (March 5th) The Rector Research Prize of the Hebrew University.
- 2012 (August) The “August-Wilhelm-von-Hofmann-Denkünze (Medal)” Awarded by the German Chemical Society (GDCh) in the 4th EuCheMS in Prague, August 26-2012.
- 2013: Saerree K. and Louis P. Fiedler Chair in Chemistry.
- 2013: Selected as a **Scrocco Colloquia Lectureship** in Scuola Normale Superiore di Pisa.
- 2013: Nominated and selected to be included in “175 faces in Chemistry” (the Royal Society of Chemistry). [<http://www.rsc.org/diversity/175-faces/all-faces/professor-sas...>]
- 2013 (Dec.): **The Lu Jiayi Lectureship Award** in The State Key Laboratory, University of Xiamen, Xiamen, China.
- 2014-2015: Extension of the Alexander von Humboldt Senior Research Award
- 2015 (June): Elected member of the International Academy of Quantum Molecular Science (IAQMS).
- 2017 (February): The Gold Medal of the Israel Chemical Society
- 2018: Awarded **The Stratingh Lectureship** in the Department of Chemistry, The university of Groningen, The Netherland.
- 2018-2019: Extension of the Alexander von Humboldt Senior Research Award
- 2019 (February): Chosen as **The Platinum Jubilee Lecturer** by the CSIR – Indian Institute of Chemical Technology (IICT) Hyderabad
- 2019 (February): An honorary Lectureship in the International Conference on Advanced Chemical and Structural Biology in Chennai
- 2019 (October): **The SOLVAY Colloquium Lectureship**
The Solvay Institute, Brussels, Belgium
- 2020 (March): **The Van’t Hoff Speaker**
The PAC Symposium, Leiden, The Netherland

8. LECTURESHIPS

- 1986: The Department of Chemistry, University of Huntsville, and Huntsville Alabama.
- 1987: The Laboratoire de Chimie Theorique, Universite de Paris-Sud, France.
- 1987: The Department of Chemistry, University of Padova, Italy.
- 1988: The Kahlbaum Lectureship, The University of Basel.
- 1989: The Departments of Chemistry,
The University of Lund, Sweden.
The University of Goteborg, Sweden.
- 1990: The Laboratoire de Chimie Theorique, Universite de Paris-Sud, France.
- 1991: The Department of Chemistry, The University of Rochester, USA.
- 1996: The Department of Chemistry, The University of Rochester, USA.
- 1993: The Department of Organic Chemistry, The Technical University of Berlin, Berlin, Germany.
- 1997: The Troisieme Cycle Lecturer of the French Speaking Swiss Universities (Friebourg, Berne, Neuchatel, Geneve).
- 1998: The Austrian Chemical Society Lectureship (Vienna, Graz, Innsbruck).
- 1999: Selected the second time as A Troisieme Cycle Lecturer (University of Basel).
- 2000 (fall) Visiting Professor in the State Key Laboratory, Xiamen University, Fujian, China
- 2001 (spring) Visiting Professor in The Ecole Normal Superieur in Paris
- 2004 (Summer) The Kurt-Alder Lectureship of the University of Cologne
- 2003 (fall) Visiting Professor in the State Key Laboratory, Xiamen University, Fujian, China
- 2006 (Winter) The Christmas Lectureship of the University of Heidelberg
- 2007 (Spring) The IQCB Lectureship of the Institute of Organic Chemistry and Biochemistry of the Academy of Sciences in Prague.
- 2007 (fall) Royal Institute of Technology, School of Biotechnology (KTH) – Stockholm, Sweden
“Valence Bond Theory: Chemical Reactivity and the Nature of the Chemical Bond”
A series of 6 lectures
- 2010 (June) Leonard N. Owen Lectureship at the Imperial College, London.
- 2010 (August) Selected as the 1st Lecturer for the International Lectureship Series for Computational Science: SCILS- The University of Cape Town.
- 2013 (June): Selected as a Scrocco Lecturer in Scuola Normale Superiore di Pisa.

- 2013 (Dec.): The Lu Jiayi Lectureship in The State Key Laboratory, University of Xiamen, Xiamen, China.
- 2018 (May): The Stratingh Lectureship in the Department of Chemistry, The university of Groningen, The Netherland.
- 2019 (February): The Platinum Jubilee Lecture
CSIR – Indian Institute of Chemical Technology (IICT) Hyderabad
- 2019 (February): An honorary Lectureship in the International Conference on Advanced Chemical and Structural Biology in Chennai
- 2019 (October): The SOLVAY Colloquium
The Solvay Institute, Brussels, Belgium
- 2020 (February) The Israel Chemical Society Meeting, Jerusalem, Israel
- 2020 (March): The Van't Hoff Speaker
The PAC Symposium, Leiden, The Netherland
- 2020 (March-on) Corona Times

9. TEACHING RATINGS

- 1980-92: Selected a few times by the students as one of the best University teachers (Ben Gurion University).
- 1995: Selected by the students as one of the best University teachers (Hebrew University).

10. BIOGRAPHIES

- 1992-present: "Who is Who in Science and Engineering"
- 1997-present: "Who is Who in The World"
- 2008: Autobiography in the Journal of Physical Chemistry A.
- 2007: Biography in Wikipedia

11. UNDERGRADUATE AND GRADUATE TEACHING

UNDERGRADUATE COURSES:

- (1) General Chemistry (for Biology students, for Pharmacology students).
- (2) Quantum Chemistry of Many Electron Systems.
- (3) Organometallic Chemistry.
- (4) Chemistry as a Game of "LEGO" -- Chemistry for Social Sciences and Humanities (1992-1998; 2010-2017).

- (5) Applied Quantum Chemistry (1992-2011)
- (6) General Chemistry (introductory chemistry course).
- (7) Seminar for B.Sc. students (2007).

GRADUATE COURSES:

- (1) Molecular Orbital Theory: A General Approach to Chemical Bonding and Structure.
- (2) Valence Bond Theory: A General Approach to Chemical Bonding and Reactivity.
- (3) Topics in Organometallic Chemistry.
- (4) Reactive Intermediates in Organic Chemistry.
- (5) Applied Qualitative Quantum Chemistry.
- (6) Chapters in History of Chemistry.

12. A PARTIAL LIST OF RESEARCH STUDENTS, POSTDOCS AND ASSOCIATES

- 1982-1984: Dr. E. Aharon-Shalom. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
- 1982-1983: Dr. V.R. Kaufman. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
- 1980-1984: Mrs. R. Bar, "Volunteer Research Associate", under the auspices of Bar-Ilan University.
- 1980-1981: Dr. J.A.R.P. Sarma. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
- 1986-1988: Ms. Avital Bartuv. An Undergraduate Research Student, Ben-Gurion University.
- 1988-1989: Mr. Eyal Duzzi. An Undergraduate Research Student, Ben-Gurion University.
- 1989-1990: Dr. Jeoung-Ki Cho. A Post Doctoral Fellow, Ben Gurion University.
- 1992-4: Dr. A. Ioffe. A Senior Research Associate, Ben-Gurion and the Hebrew Universities.
- 1992-5: Dr. A. C. Reddy. A Post Doctoral Fellow (The Lady Davis Fellowship), The Hebrew University.
- 1994-6: Dr G. N. Shastry. A Post Doctoral Fellow, The Hebrew University.
- 1994-2000: Ms. A. Shurki, Graduate student, The Hebrew University.
- 1997-2000 Dr M. Filatov. A Post Doctoral Fellow, The Hebrew University
- 1996-7 Dr V. Dubnikov. A Senior Research Associate, The Hebrew University

- 1997-1999 Dr. J. Galbraith. A Post Doctoral Fellow (The Lady Davis Fellowship), The Hebrew University
- 1997-1999 Dr. N. Harris. A Post Doctoral Fellow (The Foulbright Fellowship), The Hebrew University
- 1997-9 Dr. W. Wu, A Post Doctoral Fellow, The Hebrew University
- 1998-9 Dr S. -J. Zhong, A Post Doctoral Fellow, The Hebrew University
- 1999-2001 Esti Blanck, Undergraduate student.
- 1999-2000 Shimrit Cohen, Undergraduate student.
- 1999-2000 Youval Alpert, Undergraduate student.
- 1999-2002 Dr. Francois Ogliaro. A Post Doctoral Fellow, The Hebrew University
- 2000-2004 Dr. Samuel de Visser. A Post-Doctoral Fellow, The Hebrew University
- 2001-2002 Dr. Jose Kaneti. A Post-Doctoral Fellow, The Hebrew University
- 2000-2005 Shimrit Cohen. M.Sc.+Ph.D. Student, The Hebrew University
- 2000-2002 Dr. Pankaz K. Sharma, A Post-Doctoral Fellow, The Hebrew University
- 2001- 2004 Nir Nevo, Undergraduate student.
- 2001- 2003 Elina Ploschnik, Undergraduate student and a MSc student.
- 2002- 2005 Dr. Devesh Kumar, A Post-Doctoral Fellow, The Hebrew University
- 2001- 2007 Sebastian Kozuch, M.Sc. and Ph.D. Student, The Hebrew University
- 2002- 2004 Avraham Gutman. Undergraduate student.
- 2002- 2004 Tamara Niazov. Undergraduate student.
- 2003-2007 Karina Chazan, A Post-Doctoral Fellow.
- 2004 Ronen Shacham. A Post-Doctoral Fellow.
- 2004-2007 Tal Kataz. Undergraduate Student
- 2004-2007 Etienne Derat. A Post-Doctoral Fellow
- 2003- 2006 Elina Ploschnik. M.Sc. student, the Hebrew University.
- 2005-2008 Hajime Hirao. A Post-Doctoral Fellow.
- 2005- 2009 Kyung-Bin Cho. A Post-Doctoral Fellow.
- 2006-2009 Maria-Angels Carvajal Barba. A Post-Doctoral Fellow.
- 2006-2007 Yohann Moreau. A Post-Doctoral Fellow.

- 2006-2009 Chen Hui. A Post-Doctoral Fellow.
- 2005-2009 Dan Fishelovitch. A Ph.D. student.
- 2007-2009 N. Jena. A Post-Doctoral Fellow.
- 2007-2010 Y. Wang. A Post-Doctoral Fellow.
- 2007-2009 Rinat Meir. An M.Sc. student
- 2009-2011 Dr. Patrick Schyman, A Post-Doctoral Fellow
- 2008-2011 Dr. W. Lai. A Post-Doctoral Fellow
- 2009-2011 Dr. Deepa Janardanan, A Post-Doctoral Fellow
- 2009: Jinshuai Song. A Ph.D. student (from Xiamen, supported by the Chinese Government for 1 year)
- 2009: A. Uhe. A Ph.D. student (from Univ. of Aachen, for 3 months)
- 2009: Jorge Echeverria Lopez. A Ph.D. student (from the Univ. of Barcelona, for 3 months)
- 2009-2014: Dr. Usharani Dandamundi. A Postdoctoral Fellow.
- 2010: M. Podewski. A PhD student from the ETH (for 1 month).
- 2010-2011: Dr. Petr Milko. A Post-Doctoral Fellow (from the Institute of Organic Chemistry and Biochemistry, Prague)
- 2010-2013 Dr. Chunsen Li. A Post-Doctoral Fellow (from Xiamen University).
- 2010-2012: Dr. Mugesh Chourasia. A Postdoctoral-Fellow (from IICT Hyderabad).
- 2012: Prof. Carroll Parish, 4 month Sabbatical as a Fulbright Fellow
- 2012-3: Dr. Soumen Saha. A PBC Post-Doctoral Fellow
- 2012-2016: Dr. Binju Wang. A PBC Post-Doctoral Fellow
- 2012-3: Dr. D. Senthilnathan. A PBC Post-Doctoral Fellow
- 2013-2017: Dr. Debasish Mandal. A Post-Doctoral Fellow
- 2013-2017: Dr. Rajeev Ramanan. A PBC Post-Doctoral Fellow
- 2013-2014: Dr. Changwei Wang (Xiamen University). A Post-Doctoral Fellow
- 2013: Jing Huang. An Exchange Student for 3 months.
- 2014: David Stevens. An Exchange Student for a semester

- 2014-2017: Dr. Kshatresh D. Dubey. A PBC Post-Doctoral Fellow
- 2014-2017: Dr. Dibyendu Mallick. A PBC Post-Doctoral Fellow.
- 2015-2016: Dina A. Sharon. A Fulbright Student from Princeton
- 2015-2017: Dr. Jing Huang (Xiamen University). A Post-Doctoral Fellow.
- 2016-2017: Dr. Saritha Banda, A Post-Doctoral Fellow
- 2016-2017: Croix J. Laconsay. A Fulbright Student from Marist College
- 2017-2019: Dr. Su Hao. A Post-Doctoral Fellow
- 2017-2019: Dr. Zhanfeng Wang. A Post-Doctoral Fellow
- 2017-present: Dr. Chao Wang. An Exchange (CSC-HU exchange program) Ph.D. Student from the Academy of Science in Beijing.
- 2018-2021: Dr. Thijs Stuyver (Free University of Brussles). A Post-Doctoral Fellow.
- 2018-2021: Dr. Joy Jyothish (University of Hyderabad). A Post-Doctoral Fellow.
- 2019-2020: Dr. H. Kisan Kumar (IIT Mumbai). A Post-Doctoral Fellow
- 2019-present: Dr. Totan Mondal. A PBC Post-Doctoral Fellow
- 2019-present: Dr. Nishamole Kuriakose. A PBC Post-Doctoral Fellow
-
- 1982-1984: Dr. E. Aharon-Shalom. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
- 1982-1983: Dr. V.R. Kaufman. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
- 1980-1984: Mrs. R. Bar, "Volunteer Research Associate", under the auspices of Bar-Ilan University.
- 1980-1981: Dr. J.A.R.P. Sarma. Post Doctoral Fellow, Ben Gurion University (jointly with S. Bittner, J. Bernstein and J.Y. Becker from BGU).
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- 1988-1989: Mr. Eyal Duzzi. An Undergraduate Research Student, Ben-Gurion University.
- 1989-1990: Dr. Jeoung-Ki Cho. A Post Doctoral Fellow, Ben Gurion University.
- 1992-4: Dr. A. Ioffe. A Senior Research Associate, Ben-Gurion and the Hebrew Universities.

- 1992-5: Dr. A. C. Reddy. A Post Doctoral Fellow (The Lady Davis Fellowship), The Hebrew University.
- 1994-6: Dr G. N. Shastry. A Post Doctoral Fellow, The Hebrew University.
- 1994-2000: Ms. A. Shurki, Graduate student, The Hebrew University.
- 1997-2000 Dr M. Filatov. A Post Doctoral Fellow, The Hebrew University
- 1996-7 Dr V. Dubnikov. A Senior Research Associate, The Hebrew University
- 1997-1999 Dr. J. Galbraith. A Post Doctoral Fellow (The Lady Davis Fellowship), The Hebrew University
- 1997-1999 Dr. N. Harris. A Post Doctoral Fellow (The Foulbright Fellowship), The Hebrew University
- 1997-9 Dr. W. Wu, A Post Doctoral Fellow, The Hebrew University
- 1998-9 Dr S. -J. Zhong, A Post Doctoral Fellow, The Hebrew University
- 1999-2001 Esti Blanck, Undergraduate student.
- 1999-2000 Shimrit Cohen, Undergraduate student.
- 1999-2000 Youval Alpert, Undergraduate student.
- 1999-2002 Dr Francois Ogliaro. A Post Doctoral Fellow, The Hebrew University
- 2000-2004 Dr Samuel de Visser. A Post Doctoral Fellow, The Hebrew University
- 2001-2002 Dr Jose Kaneti. A Post Doctoral Fellow, The Hebrew University
- 2000-2005 Shimrit Cohen. M.Sc.+Ph.D. Student, The Hebrew University
- 2000-2002 Dr Pankaz K. Sharma, A Post Doctoral Fellow, The Hebrew University
- 2001- 2004 Nir Nevo, Undergraduate student.
- 2001- 2003 Elina Ploschnik, Undergraduate student and a MSc student.
- 2002- 2005 Dr Devesh Kumar, A Post Doctoral Fellow, The Hebrew University
- 2001- 2007 Sebastian Kozuch, MSc and PhD Student, The Hebrew University
- 2002- 2004 Avraham Gutman. Undergraduate student.
- 2002- 2004 Tamara Niazov, Undergraduate student (to become shortly M.Sc. student).
- 2003-2007 Karina Chazan, A Post Doctoral Fellow.
- 2004 Ronen Shacham, A Post Doctoral Fellow.
- 2004-2007 Tal Kataz, Undergraduate Student

- 2004-2007 Etienne Derat, A Post Doctoral Fellow
- 2003- 2006 Elina Ploschnik, M.Sc. student, The Hebrew University.
- 2005-2008 Hajime Hirao, A Post Doctoral Fellow.
- 2005- 2009 Kyung-Bin Cho, A Post Doctoral Fellow.
- 2006-2009 Maria-Angels Carvajal Barba, A Post Doctoral Fellow.
- 2006-2007 Yohann Moreau, A Post Doctoral Fellow.
- 2006-2009 Chen Hui, A Post Doctoral Fellow.
- 2005-2009 Dan Fishelovitch, a PhD student.
- 2007-2009 N. Jena, A Post Doctoral Fellow.
- 2007-2010 Y. Wang, A Post Doctoral Fellow.
- 2007-2009 Rinat Meir, An MSc student
- 2009-2011 P. Schyman, A Post Doctoral Fellow
- 2008-2011 W. Lai, A Post Doctoral Fellow
- 2009-2011 D. Janardanan, A Post Doctoral Fellow
- 2009: J. Song, a PhD student (from Xiamen, supported by the Chinese Government for 1 year)
- 2009: A. Uhe, a PhD student (from Univ. of Aachen, for 3 months)
- 2009: J. Echeverria Lopez (from the Univ. of Barcelona, for 3 months)
- 2009-2014: U. Dandamundi, A Postdoctoral Fellow.
- 2010: M. Podewski, a PhD student from the ETH (for 1 month).
- 2010-2011: P. Milko (from the Institute of Organic Chemistry and Biochemistry, Prague)
- 2010-2013 C. Li, a Postdoctoral Fellow (from Xiamen University).
- 2010-2012: M. Chourasia a Postdoctoral Fellow (from IICT Hyderabad).
- 2012: Prof. Carroll Parish, 4 month Sabbatical as a Fulbright Fellow
- 2012-3: S. Saha, A PBC Postdoctoral Fellow
- 2012-2016: B. Wang, A PBC Postdoctoral Fellow
- 2012-3: D. Senthilnathan, A PBC Postdoctoral Fellow
- 2013-2017: D. Mandal, A Postdoctoral Fellow

- 2013-2017: R. Ramanan, A PBC Postdoctoral Fellow
- 2013-2014: C. Wang, A Postdoctoral Fellow
- 2013: Jing Huang An Exchange Student for 3 months.
- 2014: D. Stevens, An Exchange Student for a semester
- 2014-2017: K.D. Dubey. A PBC Postdoctoral Fellow
- 2014-2017: D. Mallick, A PBC Post Doctoral Fellow.
- 2015-2016: D.A. Sharon, A Fulbright Student from Princeton
- 2015-2017: J. Huang, A Post Doctoral Fellow.
- 2016_2017 S. Banda, A Post Doctoral Fellow
- 2016-2017: Croix J. Laconsay, A Fulbright Student from Marist College
- 2017-present: S. Hao, A Post Doctoral Fellow
- 2017-present: Z. Wang, A Post Doctoral Fellow
- 2017-present: C. Wang, An Exchange (CSC-HU exchange program) Ph.D. Student from the Academy of Science in Beijing.
- 2018-present: T. Stuyver, A Post Doctoral Fellow.
- 2018-present: J. Jyothish, A Post Doctoral Fellow.
- 2019-present: H. Kisan Kumar, A Postdoctoral Fellow
- 2019-present: T. Mondal, A PBC Postdoctoral Fellow
- 2019-present: Nishamole Kuriakose, A PBC Postdoctoral Fellow

13. SUMMARY OF RESEARCH ACHIEVEMENTS (1981-ON)

Here are the major works:

(a) Valence Bond (VB) Model of Chemical Reactions: What is the origin of the barrier in chemical reactions? Why some reactions are stepwise while others are concerted single-step reactions? Is it possible to estimate barriers, solvent effects, and predict stereoselectivity, regioselectivity, and transition state (TS) structures, for a broad range of reactions in some simple and yet predictive manners? Is microscopic reversibility always obeyed? How do photochemical reactions proceed? We have created such a predictive system of thought using VB theory, which provides more accessible insight into reactivity than other theories (e.g., molecular orbital theory, or DFT). While doing so, I also revived VB theory and projected its beauty and utility to the community.

The chemical-reactivity work started in 1981 and has ever since been published well over 100 papers, reviews and two books, in which I demonstrated the wide-ranging and unified applicability of the model, from simple reactions like $H + H_2$, through organic reactions and reaction mechanisms, and all the

way to reactivity and mechanisms of metallo-enzymes. All this insight is gained using just two types of VB diagrams. The spine of the diagram is the avoided crossing of the principal VB-state curves, which describe the interchange of the bonds in reactants and products during the transformation. The avoided crossing creates a barrier, with a height that is proportional to the promotion energy gap between the state curves at the reactants' and products' geometries. The avoided crossing energy term (coupling between the state-curves) determines the stereochemistry and structure of the TS. There are other excited states, which can either mix into the TS of the concerted reaction, or fall below the crossing point of the principal curves and thereby generate reaction intermediates. These VB diagrams provide additionally a link between thermal and photochemical reactions, and enable one to derive the chemical structures of conical intersections as a general mechanism for photochemistry. Despite the theoretical rigor of the model, it achieves all this insight in a pictorial and an easy-to-use manner. The recent VB treatments of the reactions catalyzed by Cytochrome P450, and of hydrogen-atom transfer (HAT) reactivity across the board including a derivation of a predictive expression for identity H-abstraction barriers, and the unification of HAT and proton-coupled electron transfer (PCET), demonstrate the versatility and unifying power of this model.

(b) A New Outlook of the Chemical Icon Benzene and Electronic Delocalization: Benzene is a chemical icon, and most chemists believe that it has a uniform D_{6h} symmetry and special stability because the π -electrons prefer to be delocalize and hence driving the molecule to adopt a D_{6h} symmetric structure. In 1984 I questioned this dogma and showed that for any number of electrons that can undergo delocalization in a uniform symmetric structure, one could find a series of isoelectronic species in which the delocalized species are either unstable TSs or stable-delocalized clusters. The nature of these species can be predicted from the promotion energy gap in the corresponding VB diagram traced along the localizing distortion. When this promotion-energy quantity is large, as in H_2 , all the uniform H_n species (e.g., $D_{6h} H_6$) will be TSs of the respective bond exchange reactions, while when this quantity is small as e.g., in Li_2 (and other metallic dimers), the Li_n species will be a stable cluster with delocalized electrons. I showed that this promotion-energy quantity is large for π -bonds, and *therefore all the delocalized π -electronic systems like the one in benzene must behave like TSs, trapped by their frames of sigma-bonds in uniform-symmetric structures* (e.g., D_{6h} benzene). My co-workers [primarily Hiberty from Orsay] and I have changed the view on these chemical icons and showed that these π -species possess a duality; on the one hand the π -delocalization stabilizes the molecule, and on the other, they behave as distortive π -TSs trapped and blocked by their sigma frames.

I then went a step further, and showed that the distortivity of these π -TSs causes their twin-excited states (which arise due to avoided crossing along the localizing coordinate) to possess an exalted frequency of the localized mode. Thus, if you disrupt the delocalized π -electrons of benzene by exciting it to the ${}^1B_{2u}$ excited state you will find that the b_{2u} mode is selectively exalted from 1309 to 1570 cm^{-1} . You weaken π -bonding and the frequency increase, quite surprising! *This new outlook completely changed the understanding of these molecules and opened new vistas to their unique twin-excited states, and provided a link between Kekulé structures and experimental observables.*

(c) Entangled Reactivity and Breakdown of Microscopic Reversibility: My coworkers and I questioned the outer-sphere electron transfer mechanism in molecular chemistry and developed the alternative bonded electron-transfer model. We demonstrated that this model brings about entangled-reactivity, which *leads to the breakdown of microscopic reversibility*. Electron transfer (ET) reactions have a common set of VB states as the respective 'polar reactions' in which bonds are broken and made. Starting 1995, we have shown that the VB mixing and avoided crossing of these states for reactions of donors (nucleophiles) and acceptors (electrophiles) are completely entangled. Consequently, a series of

reaction will exhibit mechanistic crossover from ‘polar’ to ET reactions, and in the intermediate region of this crossover, the TSs will be common for both mechanisms, such that *a single TS will serve two mechanism and will lead to two different products, in violation of microscopic reversibility*. In fact, entangled reactivity and breakdown of microscopic reversibility should be common, and are expected whenever two mechanisms share a common set of VB-states (e.g., SN1-SN2, E1-E2-E1_{cb}, etc.)

(d) Two-State Reactivity (TSR) and Multi-State Reactivity (MSR) in Bioinorganic and Enzymatic Chemistry: In 1994 I shifted my interest to reactions of transition metal complexes, which are important in oxidative chemistry of metallo-enzymes, like Cytochrome P450. These complexes have a variety of different spin- and electromeric states, which are either degenerate or condensed into a small energy span. There were puzzles but no answers or models to comprehend these puzzles and predict their patterns. For example, why was FeO⁺ a very poor oxidant for H₂ despite the fact that the reaction was spin conserving, highly exothermic, and had no symmetry or other restriction on the reaction? What was the reason that the oxidation of alkane by P450 proceeded in a stepwise reaction via radical intermediates, despite the available very exothermic concerted pathway? And why these intermediates had lifetimes shorter than those of transition states? We have shown that the reactions proceeded on different spin-state surfaces, and this two-states reactivity (TSR) leads to immediate solutions of these puzzles. Thus, for example, the two states in P450 are parallel roots, one of which leads to normally lived radicals and the other to effectively concerted reactions (with zero radical lifetime). Consideration of TSR and MSR scenarios enriches the scope of chemical reactivity patterns and opens up a new mechanistic territory on the role of spins in chemical reactivity. Furthermore, spin-state crossing results in internal catalysis of many bioinorganic reactions. These ideas and many others were published in several reviews and reoriented the field and defined its cutting edge.

(d) New Reactivity paradigms: Exchange-Enhanced Reactivity (EER): Why does nature use nonheme iron enzymes with active species in a high-spin ($S = 2$) electronic configuration? This puzzle has been posed by the alpha-ketoglutarate mediated nonheme enzymes, which can bring about the activation of the strongest of C-H bonds (e.g. in methane and taurine). Addressing this puzzle by my coworkers and I resulted in the formulation of *the EER principle of reactivity*. Thus, we showed that when the enzyme activates the C-H bond, this enriches the metal’s d-block orbitals by a single electron. In the high-spin state, e.g. $S=2$ of Fe^vO complexes, with four identical-spin electrons, this added electron *goes into a vacant d-orbital and causes a dramatic increase the exchange-interaction*. This results in lowering of electron-electron repulsion (by ca. 50 kcal/mol) and a drastic lowering of the reaction barrier. By contrast, on lower spin-states, the exchange is depleted and the barriers are high. The derivation of the EER principle was shown to be attended orbital selection rules, which control the structure of the TS. The EER concept emerges as a key principle for understanding the origins of spin-state selectivity, and the reason why nature has selected nonheme enzymes with an $S = 2$ state, which proceeds via the EER pathway. EER is a chemical law of nature!

(f) New Bonding paradigms: Charge-Shift Bonding (CSB): The conceptual element from which an entire chemical universe can be constructed is the chemical bond. As such, the bond is the “quantum building block” of the grand scheme of “LEGO” by which practicing chemists devise and control the formation of new molecules of ever increasing complexity and beauty. My collaborators (foremost, Hiberty) and I have pointed out that in addition to the classical covalent and ionic bonds, there exist a family of bonds that have never before been recognized. These are the charge-shift bonds (CSB) in which the binding does not arise from either the covalent- or the ionic-VB states, but from their resonance interaction (i.e. the coupling between the two VB states). Thus, whenever the atoms which engage in bonding suffer a steep rise in the kinetic energy during the process (e.g., dues to atomic shrinkage in bonding, and to Pauli repulsions of the bond with lone pairs or other bond pairs), the bonding will be

brought about by charge-shift resonance, since this coupling term contributes “negative kinetic energy” that enables to restore the virial ratio and establish a bond in equilibrium. CSBs occur, *inter alia*, for electronegative and lone-pair rich atoms (e.g., in F_2), and for bonds the inverted bond in [1.1.1] propellane that are subject to large Pauli repulsion. We have shown that CSBs have experimental manifestations and the charge-shift resonance energy can even be quantified from experiments. The work will change the mental map of the chemical bond.

(g) The Triplet Bond - Bonding of Parallel Spins: Ever since 1999, I began to describe no-pair ferromagnetic (NPFM) bonds that hold together monovalent metallic atoms using exclusively parallel spins. Thus, without any traditional electron-pair-bonds, the bonding energy per two atoms in these clusters can nevertheless reach 40 kcal mol⁻¹! The VB modeling shows that this bonding motif arises from *bound triplet electron pairs* (hence may be called, the **Triplet Bond**) that are delocalized over all the close neighbors of a given atom in the cluster. The VB model shows the origins of the tendency of NPFM clusters to assume polyhedral shapes with rather high symmetry, and for the very steep rise of the bonding energy with cluster size. The advent of NPFM clusters offers new horizons in chemical bonding, and in chemistry of highly magnetic species, sensitive to magnetic and electric fields.

(h) Quadruple Bonds in Carbon and Other 1st Row Main Elements: Recently, we showed that C_2 and other isoelectronic species break the glass ceiling of multiple bonding and have quadruple bonds. This changes a fundamental dogma in chemistry, which is rooted in the early 20th century.

(i) Weak Intermolecular Interactions: My coworkers and I have developed VB-based models which lead to a lucid understanding of weak interactions, which glue mesoscopic and macroscopic materials, such as dihydrogen interactions and halogen-bonds”.

Among the many other achievements, our group made fundamental contributions to understanding of catalytic cycles, usage of KIEs and tunneling to probe the identity of the reactive spin state in enzymatic and bioinorganic H-abstractions.

(j) Oriented External Electric Fields as Tweezers and Catalysts: the usage of oriented external electric field as catalysts and means of control in chemical and enzymatic reactivity, and finding a new mechanism of DNA repair, which was spotlighted by the journal.

OLDER-DETAILED SUMMARY OF RESEARCH ACHIEVEMENTS 1981-ON

(a) 1981-2011: A valence bond approach to reactivity.

- The work started with a theoretical paper, published in 1981 and has evolved throughout the years into a unified system of thought about chemical reactivity, summarized in reviews, chapters and books. The works has been incorporated into textbooks and have led to revival of VB theory in chemistry.
 - The work was characterized by R. Hoffmann as a main contribution to the renaissance in valence bond theory (R. Hoffmann, Chemistry in Britain, March 1991, Letters section).
 - The VB model has been incorporated into a leading text book, T.H. Lowry, S. Richardson, “Mechanism and Theory in Organic Chemistry”, 3rd Ed 1987 (introductory page ix, and pp 218-223, 229, 354-360, 371, 381-382, 412, 604-608, 659, 685, 769).
 - The VB model has been incorporated into a leading monograph, L. Ebersson, “Electron Transfer Reactions in Organic Chemistry”, 1987 (pp 8 (the model is introduced as “An alternative to the Marcus model...”) pp, 23-25, 95, 141-142, 193).
 - The work has been incorporated into an advanced organic chemistry text, 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).
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(b) Bonded Electron Transfer Transition States and Selection Rules.

- The work started with a derivation of orbital selection rules for transition states of electron transfer reactions vis-à-vis their bond making analogs. Its application in the reactivity of radical anions has resulted in exciting results that are entirely different than those predicted by the outer-sphere theory of Marcus. These results involve entangled reactivity and breakdown of microscopic reversibility through surface bifurcation.
 - The work has been reviewed recently in the highlight section of *Angewandte Chemie: H. Zipse, Angew. Chem. Int. Edit. Engl.* **1997**, *36*, 1697.
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(c) Is electronic delocalization a driving force of bonding and structure?

- The work has started in a 1984 paper, which tried to provide a unified model for assessing the stability of delocalized clusters and species. It turns out that one can conceptualize all these species, stale clusters all the way to transition states of chemical reactions using a single organizing quantity, the promotion energy gap in the VB diagram. Based on this it was possible to predict that the π -electronic components of molecules like benzene, allyl and so on are transition states that are trapped by their σ -frames in structures with uniform C-C bond lengths, and are delocalized only because of this constraint. The model was extended to the twin-excited states and led to the development of structural and spectroscopic probes of the distortivity. To cite a recent introduction to a thematic issue of *Chemical Reviews*: “The once controversial idea that the geometry of benzene and other molecular icons is determined by the σ -frame, while the π -electronic system in fact prefers a distorted geometry has become widely accepted” (P.v.R Schleyer, *Chem. Rev.* **2001**, *101*, 1117).
 - The work has been reviewed as a highlight in CHEMTRACTS: J. K. Burdett, CHEMTRACTS- INORGANIC CHEMISTRY, **1991**, *3*, 57-61.
 - 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 (“perhaps we should take some aspects of chemical bonding, each of importance to chemists and study them 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?”).
 - The work has been mentioned in the letters section of C&E News, April 4, 1996 (p 4, “Proper Benzene Citation” by, R. Hoffmann and J. P. Dinnocenzo).
 - The work has been highlighted in C&E News in the section Science/Technology Concentrates, November 3, 1997 (p 21, “Benzene from a different view”).
 - The work has been reviewed in *J. Chem. Educ.* (Heilbronner, E. *J. Chem. Ed.* **1989**, *66*, 471, and Mulder (*J. Chem. Ed.*, **1998**, *75*, 594).
 - The work was reviewed in a recent paper of history of chemistry, S.G. Brush, “Dynamics of Theory Change in Chemistry: The Benzene Problem”. Part I, *Studies in History and Philosophy of Science*, **1999**, *30*, 21; **1999**, *30*, 263
 - The work has been incorporated into an advanced organic chemistry text, F. Carroll, “Perspectives on Structure and Mechanism in Organic Chemistry”, 1995.
 - The work has been incorporated into advanced monographs on aromaticity: P.J. Garrat, “Aromaticity”, Wiley, 1986, and Minkin, V.; Simkin, B.; Glukhotsev, M., “Aromaticity and Antiaromaticity”, Wiley: New York, 1994.
 - The work will be incorporated into the 4th edition (work already in progress) of an organic chemistry textbook, K.P.C. Vollhardt, N.E. Schore, “Organic Chemistry. Structure and Function”, W.H. Freeman.
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(d) The Twin-States Concept

- 1981: Development of a general reactivity model that highlighted the importance and generality of the excited state that is the twin of the transition state.
 - 1996-1998: Development of ideas associated with transition state spectroscopy.
 - 1996: The twin-states are made from the same electronic constituents and likely to possess coincident geometries. For a given transition state there should exist a twin-excited state that is bound along the reaction coordinate (of the ground state reaction). This twin-excited state, which possesses a coincident geometry with the transition state, provides the entry and means to obtain spectral information on the transition state.
 - 1998: Demonstration (with S. Zilberg, Y. Haas) that the transition state for the semibullvalene rearrangement possesses a twin-state at a coincident geometry and the reaction coordinate mode is positive and has an exalted frequency.
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(e) Development of new bonding paradigms and prediction of their chemical manifestations:

- 1992-2013 (with P.C. Hiberty): Charge-shift is a bonding form, which was discovered by computational means, and is neither covalent nor ionic. The bonding is sustained totally by the resonance between the two forms. This bonding flavor characterizes both homo-nuclear bonds (F-F, O-O, N-N etc) and heteronuclear bonds (Si-Cl, etc), and appears to be the most ubiquitous bonding mechanism in chemistry. It is manifested in the behavior in condensed phase (e.g., the ever elusive silicenium ion), and is responsible for the aggregation of higher-row elements in hypercoordinated species, and for the observation of bonds with “no density”.
 - 1999-2013: Ferromagnetic bonding is a bonding form, which is responsible for the stability of high-spin clusters of alkali metals, which possess no electron pairs. It is also called “No Pair Bonding”. The bonding energy increases with cluster size and can sustain large magnetic clusters.
 - 2006: A theoretical demonstration that the covalent-ionic resonance energy of bonds is a measurable quantity.
 - 2010-2011: A demonstration that the inverted C-C bond in [1.1,1] propellane is a charge shift bond. Showing that 16 C-C bonds fall into two groups, one classically covalent, the other charge-shifted.
 - 2012: Demonstration that main elements form quadruple bonding. The strength of the 4th bond in C₂, was quantified from experiment.
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(g) Development of valence bond methods.

- 1998-present (with W. Wu): Two methods were developed in which the valence bond (VB) energy is scaled to that of density functional theory. In this manner, one obtains methods, which, on the one hand, include dynamic electron correlation (absent from most VB methods), and on the other hand, are economical in terms of computing time and enabling thereby application to large molecules (e.g., C₃₀H₃₂) and to excited states.
 - Development (with W. Wu) of advanced but economical VB methods; VBCI, VBPTn, and VBPCM, capable of treating reactions in solution.
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(f) Developing the concept of the TSR (two-state reactivity concept) in catalytic C-H/C-C bond activation by metal Oxo reagents (with H. Schwarz and D. Schroeder).

The TSR concept was developed as an answer to a set of puzzling reactivity patterns in the activation of H-H and C-H bonds by FeO⁺ and other metal-oxo cations. The initial ideas developed into a wide-ranging paradigm in bond activation.

- The TSR concept was reviewed in the highlight section of *Angewandte Chemie*, D.A. Plattner, *Angew. Chem. Int. Edit. Engl.*, **1999**, 38, 82.

- The concept paper, which introduced two-state reactivity into the enzyme field, was chosen as among the 20 most highly cited concept papers since the establishment of the journal *Chemistry – A European Journal*.
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(g) A Theory of Reactivity of Cytochrome P450 and Heme Enzymes:

- Since 1998 and on, I introduced two new paradigms into the field: **(i) two-state reactivity (TSR)**, whereby the different spin states of the active species produce different products in predictable proportion. This paradigm has already resolved a major controversy in the area of hydroxylation by P450, and is applicable to other oxidative processes, **(ii) the chameleon oxidant concept**: that describes the behavior of the active species of the enzyme, so-called Compound I that adopts its geometry and electronic structure to the specific protein environment. We postulated and demonstrated that the interaction of the protein environment with the chameleonic nature of Compound I serves as means by which the enzyme modulates its selectivity. The chameleon oxidant concept shows a potential to reorient this field of enzymatic catalysis.

- The work of the group on the mechanism of P450 hydroxylation and the structure of Compound I was highlighted in *Chemistry and Chemical Industry*, **2001**, 54-6, 680 (the Japanese equivalent of *Chem. Eng. News*).

- A recent review by one of the P450 field's leaders (P.R. Ortiz de Montellano, J.J. de Vos, *Nat. Prod.* **2002**, 19, 471-499) 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.*".

- The recent reviews of the group were selected; one (*Chem. Rev.* 1984) as one of the 6 yearly papers defined as Editor's Choice, the other (*Chem. Rev.* 2005) as "A Hot Paper Selection for the Month of November" (See: **Citing URL** - <http://www.esi-topics.com/nhp/2006/november-06-Shaik-Kumar-deVisser-Altun-Thiel.html>). During 2005-2007, paper #289 has been featured thrice in the ACS publication list of "Hot papers":

http://pubs.acs.org/journals/promo/most/hot_papers/index.html

http://pubs.acs.org/journals/chreay/promo/most/hot_papers/sept07.html

(h) 2005-2013 -Exchange-enhanced Reactivity (EER) Theory in Bioinorganic Chemistry:

EER was developed as the Hund's Rule of chemical reactivity. It has been published in numerous papers, in a Perspective in *Nature Chemistry* 2011, and in an Account in *Acc. Chem. Res.* 2013.

(i) 2012- A Theory of H-abstraction and the Mechanistic Dichotomy of Hydrogen Atom Transfer (HAT) vs. Proton-Coupled Electron Transfer (PCET):

This theory was recently developed and published in *ACIE* and in *Chemical Science*. It enables to predict barriers for HAT reactions, and it shows that how HAT reactions acquire PCET character.

(j) The derivation of "spin inversion" mechanisms in triplet organic reactions.

- 1978-1981: This work was the first attempt to handle the stereochemistry of triplet photoreactions in a uniform manner, and followed the pioneering study of Salem and Rowland on spin-orbit coupling (SOC) in organic diradicals. The SOC interaction that causes the singlet to triplet (or vice versa) transitions has been converted into molecular distortions typified by type and symmetry, and which are encoded into the stereochemistry

of the products. Many unusual features (such as formation of highly strained molecules and the heightened sensitivity to steric effects [more so than in equilibrium conditions] of triplet photochemistry) were shown to result from a blend of these mechanisms in a predictable manner.

- The theory was mentioned on p 1024 in the textbook by T.H. Lowry, S. Richardson, "Mechanism and Theory in Organic Chemistry", 3rd Ed 1987.).
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(k) Conceptualization and design of "Organic Metals"

- 1982: The electronic structure of organic metals made from donor acceptor pairs was analyzed, and the localization mechanisms in them were elucidated. The relation between an organic metal and an isomeric charge transfer complex was outlined. It was concluded that an organic metal is the thermodynamically less stable form and should be preferred under nonequilibrium conditions).
 - 1982-1992: The ideas of this work have formed a basis for the experimental research of the "Organic Metals Group" at Ben-Gurion University. The organization of the group was initiated by S. Shaik in 1982 when the field of materials and molecular devices in Israel was more or less embryonic. The key ideas of the group were outlined in a seminal 1983 paper in JACS and are still of relevance to the field of molecular electronics.
 - *The seminal study that preceded the strategic idea of preparing "molecular metals" was formulated some 15 years before the current surge of nanochemistry.*
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14. SUMMARY OF CURRENT RESEARCH ACTIVITY

Current research activity focuses on the role of tunneling to probe the identity of the reactive spin state in enzymatic and bioinorganic H-abstractions, the usage of oriented external electric field as catalysts and means of control in chemical and enzymatic reactivity and chirality, understanding mechanisms of DNA repair, chemical bonding (charting the territory of the quadruple bond in first row elements, exploring domains of CSB, and of triplet bonds), understanding the nature of weak interactions, and exploring the role of long timescale molecular dynamics simulation in predicting enzymatic selectivity.

15. POPULAR SCIENTIFIC ACTIVITIES AND HOBBIES

a) Public lectures on chemistry intended to project to the public the beauty and relevance of chemistry to mankind. Recent talk entitled: "Chemistry: A Central Pillar of Human Culture."

Has written a book for teaching chemistry: S. Shaik, *Teaching Chemistry as a Game of Construction: The Bond-Click Way*, Wiley Interscience, Hoboken, New Jersey, USA, 2016.

b) Poetry: published poems (English and Hebrew) and authored a book.

◦ English poems in "Matrix", The University of Washington Poetry Bulletin, Dec 2, 1977

◦ Hebrew poems in "Iton 77"