

List of Publications: Sason Shaik (Sason S. Shaik*)

Citations: Google Scholar (GS) [Number cit. = 57,260, H = 120 (in worldwide rankings during 2021-2023; ranked 2nd in the Hebrew University, 6th in Israel, and ~300th in the World). Worldwide Survey 2024 by ScholarGPS: "... named an inaugural Highly Ranked Scholar [0.05% of scholars worldwide]"; H = 122. 2025 ranking [0.01% of scholars worldwide] H = 125.

*At some point the initial S of my original middle name (Sabakh) was added, but was later removed

SCIENTIFIC PUBLICATIONS

June 06, 2025

1974-1975

- (1) M. Albeck, S. Shaik
"Reactions of Tellurium(IV) Halides with Anthracene and other Organic Compounds"
J. Chem. Soc. Perkin I, 1223-1229 (1975)
<https://doi.org/10.1039/P19750001223>
- (2) M. Albeck, S. Shaik
"Identification of Tellurium-Containing Compounds by Means of Mass Spectrometry"
J. Organomet. Chem., **91**, 307-313 (1975)
[https://doi.org/10.1016/S0022-328X\(00\)88997-4](https://doi.org/10.1016/S0022-328X(00)88997-4)

1977-1978

- (3) N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces"
Progr. Theor. Org. Chem., **2**, 348-369 (1977)
- (4) N.D. Epiotis, S. Shaik, J.R. Larson, F. Bernardi
"The Manifestation of Non-Bonded Attraction in the Physical Properties of Cis and Trans Olefins"
Tetrahedron, **33**, 3269-3274 (1977)
[https://doi.org/10.1016/0040-4020\(77\)80149-X](https://doi.org/10.1016/0040-4020(77)80149-X)
- (5) N.D. Epiotis, J.R. Larson, R.L. Yates, W.R. Cherry, S. Shaik, F. Bernardi
"Theory of Structural Isomerism. Vicinal vs. Geminal Homodisubstituted Molecules"
J. Am. Chem. Soc., **99**, 7460-7464 (1977)
<https://doi.org/10.1021/ja00465a011>
- (6) F. Bernardi, A. Mangini, N.D. Epiotis, J.R. Larson, S. Shaik
"The π Donating Ability of Heteroatoms"
J. Am. Chem. Soc., **99**, 7465-7470 (1977)
<https://doi.org/10.1021/ja00465a012>
- (7) N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces. 5. Sigmatropic Shifts"
J. Am. Chem. Soc., **99**, 4936-4946 (1977)
<https://doi.org/10.1021/ja00457a009>
- (8) **BOOK**
N.D. Epiotis, W. Cherry, S. Shaik, R.L. Yates, F. Bernardi
"Structural Theory of Organic Chemistry"
Top. Curr. Chem. **70**, 1-250 (1977)
- (9) F. Bernardi, N.D. Epiotis, S. Shaik, K. Mislow
"Thiacyclobutadiene and Thiabenzene: A Comparative Theoretical Analysis"
Tetrahedron, **33**, 3061-3067 (1977)
[https://doi.org/10.1016/0040-4020\(77\)80450-X](https://doi.org/10.1016/0040-4020(77)80450-X)
- (10) M. Albeck, S. Shaik
"Electrochemical Decomposition of Biformylperoxide. A Quantum Mechanical Calculation"
J. Chem. Soc., Faraday Trans.1, **74**, 1496-1499 (1978)
<https://doi.org/10.1039/F19787401496>
- (11) N.D. Epiotis, S. Shaik

- “Qualitative Potential Energy Surfaces. 1. Theory”
J. Am. Chem. Soc., **100**, 1-8 (1978)
<https://doi.org/10.1021/ja00469a001>
- (12) N.D. Epiotis, S. Shaik
 “Qualitative Potential Energy Surfaces. 2. Cycloadditions”
J. Am. Chem. Soc., **100**, 9-17 (1978)
<https://doi.org/10.1021/ja00469a002>
- (13) S. Shaik, N.D. Epiotis
 “Qualitative Potential Energy Surfaces. 3. Stereoselection Rules for Spin Inversion in Triplet Photochemical Reactions”
J. Am. Chem. Soc., **100**, 18-29 (1978)
<https://doi.org/10.1021/ja00469a003>
- (14) N.D. Epiotis, S. Shaik
 “Qualitative Potential Energy Surfaces. 4. Aromatic Substitution”
J. Am. Chem. Soc., **100**, 29-33 (1978)
<https://doi.org/10.1021/ja00469a004>
- (15) F. Bernardi, W. Cherry, S. Shaik, N.D. Epiotis
 “Structure of Fluoromethyl Radicals. Conjugative and Inductive Effects”
J. Am. Chem. Soc., **100**, 1352-1356 (1978)
<https://doi.org/10.1021/ja00473a004>
- (16) THESIS
 S.S. Shaik
 “Spin Inversion in Triplet Reactions”
 Ph.D. Dissertation, University of Washington, 1978.
 University Microfilms, 300 N. Zeeb Road, Ann Arbor, Michigan 48106, USA

1979-1980

- (17) S.S. Shaik
 “Spin-Inversion and Orbital Symmetry Conspiracy in Type A Lumiketone Rearrangements”
J. Am. Chem. Soc., **101**, 2736-2738 (1979)
<https://doi.org/10.1021/ja00504a044>
- (18) S.S. Shaik
 “Triplet (2 + 2) Cycloadditions. Spin Inversion Control of Stereoselectivity”
J. Am. Chem. Soc., **101**, 3184-3196 (1979)
<https://doi.org/10.1021/ja00506a009>
- (19) S.S. Shaik, N.D. Epiotis
 “Spin Inversion in Triplet Diels-Alder Reactions”
J. Am. Chem. Soc., **102**, 122-131 (1980)
<https://doi.org/10.1021/ja00521a022>
- (20) S. Shaik, R. Hoffmann
 “Why Some Binuclear Complexes Bridge, While Others, Even Though They Might Have a Quadruple Bond Available to Them, Do Not?”
J. Am. Chem. Soc., **102**, 1194-1196 (1980)
<https://doi.org/10.1021/ja00523a062>
- (21) S. Shaik, R. Hoffmann, C.R. Fisel, R.H. Summerville
 “Bridged and Unbridged M_2L_{10} Complexes”
J. Am. Chem. Soc., **102**, 4555-4572 (1980)
<https://doi.org/10.1021/ja00534a001>
- (22) J.R. Larson, N.D. Epiotis, L.E. McMurchie, S.S. Shaik
 “On the Role of Spin Inversion in the Triplet Photochemistry of Benzyl Halides and Benzylammonium Salts”
J. Org. Chem., **45**, 1388-1393 (1980)
<https://doi.org/10.1021/jo01296a009>
- (23) R. Hoffmann, S. Shaik, J.C. Scott, M.-H. Whangbo, M.J. Foshee
 “The Electronic Structure of $NbSe_3$ ”
J. Solid State Chem., **34**, 263-269 (1980)
[https://doi.org/10.1016/0022-4596\(80\)90230-3](https://doi.org/10.1016/0022-4596(80)90230-3)

- (24) CHAPTER
 N.D. Epiotis, S. Shaik, W. Zander
 "Rearrangements: A Theoretical Approach" in: "Rearrangements in Ground and Excited States Vol-2"
 P. De Mayo, Ed. Academic Press,
 New York, 1980, pp 1-94

1981-1984

- (25) J.R. Larson, N.D. Epiotis, S.S. Shaik
 "A Simple Theoretical Approach to Bond Energies"
Tetrahedron, **37**, 1205-1211 (1981)
[https://doi.org/10.1016/S0040-4020\(01\)92051-4](https://doi.org/10.1016/S0040-4020(01)92051-4)
- (26) S.S. Shaik
 "What Happens to Molecules as They React? A Valence Bond Approach to Reactivity"
J. Am. Chem. Soc., **103**, 3692-3701 (1981).
<https://doi.org/10.1021/ja00403a014>
- (27) A. Pross, S.S. Shaik
 "Reactivity-Selectivity Relationships. A Quantum Mechanical Approach to Transition State Structure. Application to the S_N2 Reaction of Benzyl Derivatives"
J. Am. Chem. Soc., **103**, 3702-3709 (1981)
<https://doi.org/10.1021/ja00403a015>
- (28) S.S. Shaik, A. Pross
 "S_N2 Reactivity of CH₃X Derivatives. A Valence Bond Approach"
J. Am. Chem. Soc., **104**, 2708-2719 (1982)
<https://doi.org/10.1021/ja00374a005>
- (29) A. Pross, S.S. Shaik
 "A Qualitative Valence-Bond Approach to Organic Reactivity. Application to Elimination Reactions"
J. Am. Chem. Soc., **104**, 187-195 (1982)
<https://doi.org/10.1021/ja00365a034>
- (30) S.S. Shaik
 "On the Origins of the Barrier in the S_N2 Identity Exchange"
Nouv. J. Chim., **6**, 159-161 (1982)
- (31) A. Pross, S.S. Shaik
 "Is Charge Development a Measure of S_N2 Transition State Structure?"
Tetrahedron Lett., **23**, 5467-5470 (1982)
[https://doi.org/10.1016/0040-4039\(82\)80159-7](https://doi.org/10.1016/0040-4039(82)80159-7)
- (32) A. Pross, S.S. Shaik
 "Why Do Rate-Equilibrium Relationships Break Down?"
J. Am. Chem. Soc., **104**, 1129-1130 (1982)
<https://doi.org/10.1021/ja00368a052>
- (33) S.S. Shaik
 "On the Stability and Properties of Organic Metals and Their Isomeric Charge-Transfer Complexes"
J. Am. Chem. Soc., **104**, 5328-5334 (1982)
<https://doi.org/10.1021/ja00384a013>
- (34) S.S. Shaik, A. Pross
 "On the Origins of Reaction Barriers. Application to S_N2"
Bull. Soc. Chim. Belg., **91**, 355 (1982)
<https://doi.org/10.1002/bscb.19820910514>
- (35) S. Shaik
 "Nobel Prize in Chemistry 1981. In the Frontier of Chemical Reactions" (in Hebrew)
Mada (Science), **26**, 130-132 (1982)
- (36) S.S. Shaik, R. Bar
 "The Problem of Metal-Metal (MM) Bond Alternation in [MX₂(μ-X)_{4/2}]_∞ Chain Polymers"
Inorg. Chem., **22**, 735-743 (1983)
<https://doi.org/10.1021/ic00147a007>
- (37) H. Köppel, L.S. Cederbaum, W. Domcke, S.S. Shaik
 "Symmetry Breaking and Non-Born-Oppenheimer Effects in Radical Cations"
Angew. Chem., Int. Ed., **22**, 210-224 (1983)
<https://doi.org/10.1002/anie.198302101>

- (38) S.S. Shaik
 "α- and β-Carbon Substituent Effect on S_N2 Reactivity. A Valence Bond Approach"
J. Am. Chem. Soc., **105**, 4359-4367 (1983)
<https://doi.org/10.1021/ja00351a039>
- (39) S.S. Shaik
 "Reactivity and Reactivity-Selectivity Crossovers in S_N2"
Nouv. J. Chim., **7**, 201-203 (1983)
- (40) J.Y. Becker, J. Bernstein, S. Bittner, N. Levi, S.S. Shaik
 "Strategic Design of Organic Conductors. Structure of a Prototypical Molecule"
J. Am. Chem. Soc., **105**, 4468-4469 (1983)
<https://doi.org/10.1021/ja00351a054>
- (41) A. Pross, S.S. Shaik
 "A Qualitative Valence-Bond Approach to Organic Reactivity"
Acc. Chem. Res., **16**, 363-370 (1983)
<https://doi.org/10.1021/ar00094a001>
- (42) S. Shaik
 "Roald Hoffmann. Hercule Poirot of the Molecules. Application of Molecular Orbital Theory to the Understanding of Molecular Architecture" (in Hebrew)
Hakesher Hachimi. The Chemical Bond, **8**, 10-16 (1983)
- (43) EDITING
 Y. Apeloig, S. Shaik, Eds.
 "Application of Theory to Organic and Organometallic Molecules"
Isr. J. Chem., **23**, 1-152 (1983).
- (44) S.S. Shaik
 "Solvent Effect on Reaction Barriers. The S_N2 Reaction. 1. Application to the Identity Exchange"
J. Am. Chem. Soc., **106**, 1227-1232 (1984)
<https://doi.org/10.1021/ja00317a010>
- (45) S.S. Shaik, R. Bar
 "How Important is Resonance in Organic Species?"
Nouv. J. Chim., **8**, 411-420 (1984)

1985

- (46) S.S. Shaik, P.C. Hiberty
 "When Does Electronic Delocalization Become a Driving Force of Molecular Shape and Stability? The "Aromatic" Sextet"
J. Am. Chem. Soc., **107**, 3089-3095 (1985)
<https://doi.org/10.1021/ja00297a013>
- (47) D.J. Mitchell, H.B. Schlegel, S.S. Shaik, S. Wolfe
 "Relationships between Geometries and Energies of Identity S_N2 Transition States: The Dominant Role of the Distortion Energy and its Origins"
Can. J. Chem., **63**, 1642-1648 (1985)
<https://doi.org/10.1139/v85-276>
- (48) S.S. Shaik, P.C. Hiberty, G. Ohanessian, J.M. Lefour
 "Allylic Resonance is Forced Upon the π-System by the σ-Framework"
Nouv. J. Chim., **9**, 385-388 (1985)
- (49) P.C. Hiberty, S.S. Shaik, J.M. Lefour, G. Ohanessian
 "Is the Delocalized π-System of Benzene a Stable Electronic System?"
J. Org. Chem., **50**, 4657-4659 (1985)
<https://doi.org/10.1021/jo00223a052>
- (50) E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S. Shaik
 "A New Electron Donor: Synthesis of 2,3,6,7 Tetra(ethyltellura)tetrathiafulvalene"
Tetrahedron Lett., **26**, 2783-2786 (1985)
[https://doi.org/10.1016/S0040-4039\(00\)94911-6](https://doi.org/10.1016/S0040-4039(00)94911-6)
- (51) E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S. Shaik
 "The Synthesis, Structure and Properties of the Complex Between a New Donor, 2,3,6,7-Tetra(ethyltellura)tetrathiafulvalene (TeTeTTF) and Tetracyanoquinodimethane (TCNQ)"
Synth. Met., **11**, 213-220 (1985)
[https://doi.org/10.1016/0379-6779\(85\)90018-9](https://doi.org/10.1016/0379-6779(85)90018-9)

- (52) S.S. Shaik
 "Identity S_N2 Reactions. The Relationship between Transition State Geometry, Selectivity and the Mechanism of Solvent Action"
Isr. J. Chem., **26**, 367-374 (1985)
<https://doi.org/10.1002/ijch.198500121>
- (53) REVIEW
 S.S. Shaik
 "The Collage of S_N2 Reactivity Patterns. A State Correlation Diagram Model"
Prog. Phys. Org. Chem., **15**, 197-337 (1985)
<https://doi.org/10.1002/9780470171943.ch4>

1986

- (54) D. Cohen, R. Bar, S.S. Shaik
 "Nucleophilic Vinylic Substitution. A Theoretical Study"
J. Am. Chem. Soc., **108**, 231-240 (1986)
<https://doi.org/10.1021/ja00262a008>
- (55) S.S. Shaik
 "Intrinsic Selectivity and its Geometric Significance in S_N2 Reactions"
Can. J. Chem., **64**, 96-99 (1986)
- (56) S.S. Shaik, M.-H. Whangbo
 "Electronic and Intramolecular Structural Localizations in Conducting Organic Salts"
Inorg. Chem., **25**, 1201-1209 (1986)
<https://doi.org/10.1021/ic00228a027>
- (57) P.C. Hiberty, S.S. Shaik, G. Ohanessian, J.M. Lefour
 "The π -Distortive Propensities in Benzene and the Allyl Radical. A Reply to a Criticism"
J. Org. Chem., **51**, 3908-3909 (1986)
<https://doi.org/10.1021/jo00370a035>
- (58) E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik
 "The 1:1 Mixed Stack Complex of Tetrathiafulvalene and 2,5-Dibenzyltetracyanoquinodimethane (TTF:DBTCNQ) at 115K"
Isr. J. Chem., **27**, 375-380 (1986)
<https://doi.org/10.1002/ijch.198600056>

1987

- (59) S.S. Shaik, P.C. Hiberty, J.-M. Lefour, G. Ohanessian
 "Is Delocalization a Driving Force in Chemistry? Benzene, Allyl Radical, Cyclobutadiene, and Their Isoelectronic Species"
J. Am. Chem. Soc., **109**, 363-374 (1987)
<http://doi.org/10.1021/Ja00236A013>
- (60) S.S. Shaik
 "Nucleophilicity and Vertical Ionization Potentials in Cation-Anion Recombinations"
J. Org. Chem., **52**, 1563-1568 (1987)
<https://doi.org/10.1021/jo00384a034>
- (61) E. Canadell, S.S. Shaik
 "Potentially Conducting Organometallic Systems: the Stibaphenalenyl Series"
Inorg. Chem., **26**, 3797-3802 (1987)
<http://doi.org/10.1021/Ic00269A034>

1988

- (62) S.S. Shaik
 "How is Transition State Looseness Related to the Reaction Barrier"
J. Am. Chem. Soc., **110**, 1127-1131 (1988)
<http://doi.org/10.1021/Ja00212A021>
- (63) E. Bunce, S.S. Shaik, I.-H. Um, S. Wolfe
 "A Theoretical Treatment of Nucleophilic Reactivity in Additions to Carbonyl Compounds. Role of the Vertical Ionization Energy"
J. Am. Chem. Soc., **110**, 1275-1279 (1988)

- <https://doi.org/10.1021/ja00212a041>
- (64) J.Y. Becker, J. Bernstein, S. Bittner, N. Levi, S.S. Shaik, N. Zer-Zion
“Synthesis and Properties of Archetypical Donor-Acceptor-Donor (D₂A) Molecules”
J. Org. Chem., **53**, 1689-1694 (1988)
<https://doi.org/10.1021/jo00243a017>
- (65) J. Bernstein, S.S. Shaik
“The Wave Particle Duality. Teaching via a Visual Metaphor”
J. Chem. Educ., **65**, 339-340 (1988)
<https://doi.org/10.1021/ed065p339>
- (66) J.Y. Becker, J. Bernstein, S. Bittner, E. Harlev, J.A.R.P.Sarma, S.S. Shaik
“Preparation and Structure of 2,5-Bis-(Phenylthio)-Benzoquinone and 2,6-Bis-(Phenylthio)-Benzoquinone”
Nouv. J. Chim., **12**, 875-880 (1988)
- (67) G. Ohanessian, P.C. Hiberty, J.-M. Lefour, J.-P. Flament, S.S. Shaik
“Is Delocalization a Driving Force in Chemistry? First- and Second-Row Heteroannulens”
Inorg. Chem., **27**, 2219-2224 (1988)
<https://doi.org/10.1021/ic00286a004>
- (68) S.S. Shaik, P.C. Hiberty, G. Ohanessian, J.-M. Lefour
“When Does Electronic Delocalization Become a Driving Force of Chemical Bonding?”
J. Phys. Chem., A Feature Article, **92**, 5086-5094 (1988)
<https://doi.org/10.1021/j100329a008>
- (69) J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik
“Strategic Design of Organic Conductors. Preparation and Characterization of Electron-Donor-Acceptor Complexes with Prefixed Stoichiometry”
Synth. Met., **27**, 197-204 (1988)
[https://doi.org/10.1016/0379-6779\(88\)90144-0](https://doi.org/10.1016/0379-6779(88)90144-0)
- (70) J.Y. Becker, J. Bernstein, S. Bittner, J.A.R.P. Sarma, L. Shahal, S.S. Shaik
“The Structure of 3,3',4,4'-Tetrakis(ethyltelluro)-2,2',5,5'-tetrathiafulvalene (TTeC₂-TTF)”
Acta Crystallogr. **C44**, 1770-1772 (1988)
<https://doi.org/10.1107/S0108270188003488>
- (71) S.S. Shaik, H.B. Schlegel, S. Wolfe
“Transition State Geometries and the Magnitudes of S_N2 Barriers. A Theoretical Study”
J. Chem. Soc., Chem. Commun., 1322-1324 (1988)
<http://doi.org/10.1039/C39880001322>

1989

- (72) A. Pross, S.S. Shaik
“Structure - Reactivity Coefficients. Do They Measure Transition State Structure?”
Nouv. J. Chim., **13**, 427-434 (1989)
- (73) CHAPTER
S.S. Shaik
“A Qualitative Valence Bond Model for Organic Reactions” in “New Theoretical Concepts for Understanding Organic Reactions”
NATO ASI Series **C267**, J. Bertran, G.I. Csizmadia, Eds.
Kluwer Publ., Dordrecht, Holland, 1989
- (74) S.S. Shaik, A. Pross
“Nucleophilic Attack on Cation Radicals and Cations. A Theoretical Analysis”
J. Am. Chem. Soc., **111**, 4306-4312 (1989)
<http://doi.org/10.1021/Ja00194A023>
- (75) A. Demolliens, O. Eisenstein, P.C. Hiberty, J.M. Lefour, G. Ohanessian, S.S. Shaik, F. Volatron
“Hypercoordinated XH_{n+1} Radicals for First- and Second-Row Atoms. A Valence Bond Analysis”
J. Am. Chem. Soc., **111**, 5623-5631 (1989)
<http://doi.org/10.1021/Ja00197A019>
- (76) G. Sini, P.C. Hiberty, S.S. Shaik
“The Origins of the Different Bonding Features in SiH₅⁻ and CH₅⁻; A Valence Bond Curve Crossing Model”
J. Chem. Soc., Chem Commun., 772-774 (1989)
<http://doi.org/10.1039/C39890000772>
- (77) G. Sini, S.S. Shaik, J.M. Lefour, G. Ohanessian, P.C. Hiberty
“Quantitative Valence Bond Computation of a Curve Crossing Diagram for a Model S_N2 Reaction H⁺ +

$\text{CH}_3\text{H}^+ \rightarrow \text{HCH}_3 + \text{H}^+$
J. Phys. Chem., **93**, 5661-5665 (1989)
<http://doi.org/10.1021/J100352A007>

- (78) J.Y. Becker, J. Bernstein, S. Bittner, J.A.R.P. Sarma, S.S. Shaik
 "Structural Trends in Potential Organic Conductors Based on (Donor-CH₂)₂tetracyanoquinodimethane Molecules"
Chem. Mater., **1**, 412-420 (1989)
<https://doi.org/10.1021/cm00004a007>

1990

- (79) S.S. Shaik, E. Canadell
 "Regioselectivity of Radical Attacks on Substituted Olefins. Application of the State-Correlation-Diagram (SCD) Model"
J. Am. Chem. Soc., **112**, 1446-1452 (1990)
<http://doi.org/10.1021/Ja00160A023>
- (80) P. Maitre, P.C. Hiberty, G. Ohanessian, S.S. Shaik
 "Quantitative Valence Bond Computations of Curve-Crossing Diagrams for Model Atom Exchange Reactions"
J. Phys. Chem., **94**, 4089-4093 (1990)
<http://doi.org/10.1021/J100373A038>
- (81) G. Sini, G. Ohanessian, P.C. Hiberty, S.S. Shaik
 "Why is SiH₅⁻ a Stable Intermediate While CH₅⁻ is a Transition State? A Quantitative Curve Crossing Valence Bond Study"
J. Am. Chem. Soc., **112**, 1407-1413 (1990)
<https://doi.org/10.1021/ja00160a018>
- (82) S.S. Shaik
 "The S_N2 and Single Electron Transfer Concepts. A Theoretical and Experimental Overview"
Acta Chemica Scandinavica, **44**, 205-221 (1990)
<https://doi.org/10.3891/acta.che.scand.44-0205>
- (83) L. Ebersson, S.S. Shaik
 "Electron-Transfer Reactions of Radical Anions: Do They Follow Outer- or Inner-Sphere Mechanisms?"
J. Am. Chem. Soc., **112**, 4484-4489 (1990)
<http://doi.org/10.1021/Ja00167A055>
- (84) P. Maitre, F. Volatron, P.C. Hiberty, S.S. Shaik
 "Hypercoordination in SiH₅⁻ and SiH₅^{·-}. An Electron-Count Dependence"
Inorg. Chem., **29**, 3047-3048 (1990)
<https://doi.org/10.1021/ic00341a038>
- (85) J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik
 "New 'TE-TTF' Dimers, Aryl-Substituted TCNQ, and Quinone derivatives: Synthesis, Electrochemistry and Molecular Structure"
Pure Appl. Chem., **62**, 467-472 (1990)
<http://doi.org/10.1351/Pac199062030467>
- (86) S.S. Shaik, E. Duzzy, A. Bartuv
 "The Quantum Mechanical Resonance Energy of Transition States: An Indicator of Transition State Geometry and Electronic Structure"
J. Phys. Chem., **94**, 6574-6581 (1990)
<http://doi.org/10.1021/J100380A011>
- (87) S.S. Shaik, J.P. Dinnocenzo
 "Nucleophilic Cleavage of One-Electron σ Bonds are Predicted to Proceed with Stereoinversion"
J. Org. Chem., **55**, 3434-3436 (1990)
<https://doi.org/10.1021/jo00298a004>

1991

- (88) CHAPTER
 S.S. Shaik, P.C. Hiberty
 "Curve Crossing Diagrams as General Models for Chemical Reactivity and Structure"
 "Theoretical Models of Chemical Bonding Part 4", **4**, 269-322 (1991)
- (89) S.S. Shaik
 "The LEGO Way: Curve crossing Diagrams as General Models in Physical Organic Chemistry"

- Pure Appl. Chem.*, **63**, 195-204 (1991)
<http://doi.org/10.1351/Pac199163020195>
- (90) J.Y. Becker, J. Bernstein, S. Bittner, L. Shahal, S.S. Shaik
 "Preparation of Mono- and 1,2-Di-Bromotetrathiafulvalene (TTFBr and 1,2-TTFBr₂)"
J. Chem. Soc., Chem. Commun., 92-93 (1991)
<https://doi.org/10.1039/C39910000092>
- (91) G. Sini, P. Maître, P.C. Hiberty, S.S. Shaik
 "Covalent, Ionic and Resonating Single Bonds"
J. Mol. Struct. (THEOCHEM), **229**, 163-188 (1991)
[http://doi.org/10.1016/0166-1280\(91\)90144-9](http://doi.org/10.1016/0166-1280(91)90144-9)
- (92) J.Y. Becker, J. Bernstein, S. Bittner, Y. Giron, E. Harlev, L. Kaufman-Orenstein, D. Peleg, L. Shahal, S.S. Shaik
 "Synthesis and Structure of Molecules Containing Linked Donor and Acceptor Units, New Tellurium-TTF Derivatives and their Charge transfer Complexes"
Synth. Met., **41-43**, 2523-2528 (1991)
[http://doi.org/10.1016/0379-6779\(91\)91417-9](http://doi.org/10.1016/0379-6779(91)91417-9)
- (93) S.S. Shaik
 "Valence Bond Mixing: The 'LEGO' Way. From Resonating Bonds to Resonating Transition States"
Molecules in Natural Science and Medicine: An Encomium to Linus Pauling, Z.B. Maksic, M. E. Maksic, Eds. Ellis Horwood, London, 1991
- (94) J.K. Cho, S. Shaik
 "Electron Transfer vs Polar Mechanisms. Transition-State Structures and Properties for Reactions of a Cation Radical and a Nucleophile"
J. Am. Chem. Soc., **113**, 9890-9891 (1991)
<http://doi.org/10.1021/Ja00026A046>
- (95) S. Shaik
 "The Chemistry Between The Science of Chemistry and the Gulf War"
 Magazine "Panim" (in Hebrew)
Panim, April, 20-21 (1991)
- 1992**
- (96) S. Goldstein, G. Czapski, H. Cohen, D. Meyerstein, J.K. Cho, S.S. Shaik
 "Deamination of 2-methyl-2-propanamine Induced by Hydroxyl Radicals and Metal Ions: A Comparison between the Rates of β Elimination of Ammonia and Water"
Inorg. Chem., **31**, 798-803 (1992)
<https://doi.org/10.1021/ic00031a020>
- (97) A. Pross, S. Shaik
 "What is a Good Approximation for the Transition State of an S_N2 Reaction?"
Croat. Chem. Acta, **65**, 625-631 (1992)
- (98) E. Heilbronner, S. Shaik
 "Fluctuating Double-Bond Localization and Charge Migration in π System"
Helv. Chim. Acta, **75**, 539-556 (1992)
<http://doi.org/10.1002/Hlca.19920750214>
- (99) S. Shaik, P. Maître, G. Sini, P.C. Hiberty
 "The Charge-Shift Bonding Concept. Electron-Pair Bonds with Very Large Ionic-Covalent Resonance Energies"
J. Am. Chem. Soc., **114**, 7861-7866 (1992)
<http://doi.org/10.1021/Ja00046A035>
- (100) G. Sini, S. Shaik, P.C. Hiberty
 "Quantitative Valence-Bond Computations of Curve Crossing Diagrams for A Gas-Phase S_N2 Reactions, F⁻ + CH₃F -> FCH₃ + F"
J. Chem. Soc., Perkin Trans., 2, 1019-1025 (1992)
<http://doi.org/10.1039/P29920001019>
- (101) A. Ioffe, S. Shaik
 "Intramolecular Effects in the Cycloaddition of Three Ethylenes vs the Diels-Alder reactions"
J. Chem Soc., Perkin Trans., 2, 2101-2108 (1992)
<http://doi.org/10.1039/P29920002101>
- (102) **BOOK**
 S.S. Shaik, H.B. Schlegel, S. Wolfe
 "Theoretical Aspects of Physical Organic Chemistry. Application to the S_N2 Transition State"

Wiley Interscience, NY, 1992

1993

- (103) P.C. Hiberty, G. Ohanessian, S.S. Shaik, J.P. Flament
 “The Delocalization of π Electronic Systems as a Destabilizing Constraint Imposed by the σ -Frame. Allyl, Benzene, Cyclobutadiene and Related Heteroannulenes.”
Pure Appl. Chem., **65**, 35-45 (1993)
<http://doi.org/10.1351/Pac199365010035>
- (104) D. Danovich, Y. Apeloig, S. Shaik
 “A Reliable and Inexpensive Method for Calculating Ionization Potentials and Electron Affinities of Radicals and Molecules”
J. Chem. Soc., Perkin Trans., **2**, 321-330 (1993)
<http://doi.org/10.1039/P29930000321>
- (105) S. Goldstein, G. Czapski, H. Cohen, D. Meyerstein, S. Shaik
 “Effect of N-Alkylation on The Rate of β -Amine Elimination from transients with Cu^{II} -Carbon σ -Bonds”
J. Chem. Soc., Faraday Trans., **89**, 4045-4051 (1993)
<http://doi.org/10.1039/Ft9938904045>
- (106) Y. Apeloig, O. Merin-Aharoni, D. Danovich, A. Ioffe, S. Shaik
 “Does Hydride Ion Transfer from Silanes to Carbenium Ions Proceed via a Rate-Determining Formation of a Silicenium Ion or via a Rate Determining Electron Transfer? An ab initio Quantum Mechanical Study and Curve-Crossing Analysis”
Isr. J. Chem., **33(4)**, 387-402 (1993)
<http://doi.org/10.1002/Ijch.199300046>
- (107) A. Ioffe, S. Shaik
 “Ethane Cation-Radical Isomers and their Interconversion Pathways. Electron Shift Isomerism in Cation-Radicals”
J. Chem Soc. Perkin 2, 1461-1473 (1993)
<http://doi.org/10.1039/P29930001461>
- (108) C. Lifshitz, Y. Gotkis, A. Ioffe, J. Laskin, S. Shaik
 “Is the Tropylium (Tr^+) Formed from Toluene at Its Thermochemical Threshold?”
Int. J. Mass Spectrom. Ion Processes, **125**, R7-R11 (1993)
[http://doi.org/10.1016/0168-1176\(93\)80020-F](http://doi.org/10.1016/0168-1176(93)80020-F)
- (109) C. Lifshitz, Y. Gutkis, J. Laskin, A. Ioffe, S. Shaik
 “Threshold Formation of Benzylum (Bz^+) and Tropylium (Tr^+) From Toluene. Nonstatistical behavior in Franck-Condon Gaps”
J. Phys. Chem., **97**, 12291-12295 (1993)
<https://doi.org/10.1021/j100149a032>
- (110) EDITING
 Y. Apeloig, S. Shaik, Eds.
 “Computational Quantum Chemistry- A Cornerstone of Chemical Research”, Honoring 1992 Wolf Prize Recipient John A. Pople.
Isr. J. Chem., **33, part A** 339-351 (1993).
- (111) Y. Apeloig, S. Shaik, Eds.
 “Computational Quantum Chemistry- A Cornerstone of Chemical Research”, Honoring 1992 Wolf Prize Recipient John A. Pople.
Isr. J. Chem., **33, part B** 353-457 (1993).

1994

- (112) S. Shaik
 “A Primer for Valence Bond Mixing and Avoided Crossing: General Paradigms in Chemical Reactivity”
J. Mol. Liq., **61**, 49-79 (1994)
[http://doi.org/10.1016/0167-7322\(94\)00753-5](http://doi.org/10.1016/0167-7322(94)00753-5)
- (113) S. Shaik, A. Ioffe, A.C. Reddy, A. Pross
 “Is the Avoided Crossing State A Good Approximation for the Transition State of A Chemical Reaction? Menshutkin and Ionic $\text{S}_{\text{N}}2$ Reactions”
J. Am. Chem. Soc., **116**, 262-273 (1994)

- (114) <http://doi.org/10.1021/Ja00080A030>
S. Shaik, A.C. Reddy
“Transition States, Avoided crossing States and Valence-Bond Mixing: Fundamental Reactivity Paradigms”
J. Chem. Soc., Faraday Trans., **90**, 1631-1642 (1994)
<http://doi.org/10.1039/Ft9949001631>
- (115) A. Fiedler, D. Schröder, S. Shaik, H. Schwarz
“Electronic Structures and Gas-Phase Reactivities of Cationic Late-Transition-Metal Oxides”
J. Am. Chem. Soc., **116**, 10734-10741 (1994)
<https://doi.org/10.1021/ja00102a043>
- (116) J. Blum, M.S. Fichman, L. Efron, S. Shaik, R.G. Harvey
“On the Regioselectivity in Transformation of benzo[*a*]pyrene 4,5-Oxide and 3-Methylcholanthrene 11,12-Oxide to the Corresponding β -Amino-Alcohol Derivatives”
Tetrahedron Lett., **50**, 8505-8514 (1994)
[https://doi.org/10.1016/S0040-4020\(01\)85570-8](https://doi.org/10.1016/S0040-4020(01)85570-8)
- (117) U. Samuni, S. Kahana, R. Fraenkel, Y. Haas, D. Danovich, S. Shaik
“The ICN-INC System: Experiment and Quantum Chemical Calculations”
Chem. Phys. Lett., **225**, 391-397 (1994)
[http://doi.org/10.1016/0009-2614\(94\)87100-0](http://doi.org/10.1016/0009-2614(94)87100-0)
- (118) A. Waldman, S. Ruhman, S. Shaik, G.N. Sastry
“Coherent Photochemistry in Solution. Impulsive Photoselective Photolysis of $\text{Mn}_2(\text{CO})_{10}$ ”
Chem. Phys. Lett., **230**, 110-116 (1994)
[http://doi.org/10.1016/0009-2614\(94\)01123-0](http://doi.org/10.1016/0009-2614(94)01123-0)

1995

- (119) S. Shaik, A.C. Reddy, A. Ioffe, J.P. Dinnocenzo, D. Danovich, J.K. Cho
“Reactivity Paradigms: Transition State Structure, Mechanisms of Barrier Formation, and Stereospecificity of Nucleophilic Substitutions on σ -Cation Radicals”
J. Am. Chem. Soc., **117**, 3205-3222 (1995)
<https://doi.org/10.1021/ja00116a025>
- (120) REVIEW
S. Shaik, P.C. Hiberty
“Valence Bond Mixing and Curve Crossing Diagrams in Chemical reactivity and Bonding”
Adv. Quant. Chem., **26**, 99-163 (1995)
[http://doi.org/10.1016/S0065-3276\(08\)60112-4](http://doi.org/10.1016/S0065-3276(08)60112-4)
- (121) P.C. Hiberty, D. Danovich, A. Shurki, S. Shaik
“Why Does Benzene Possess a D_{6h} Symmetry? A Quasiclassical State Approach for Probing π -Bonding and Delocalization Energy”
J. Am. Chem. Soc., **117**, 7760-7768 (1995)
<http://doi.org/10.1021/Ja00134A022>
- (122) D. Danovich, J. Hrusák, S. Shaik
“Ab Initio Calculations for Small Iodo Clusters. Good Performance of Relativistic Effective Core Potentials”
Chem. Phys. Lett., **233**, 249-256 (1995)
[http://doi.org/10.1016/0009-2614\(94\)01451-Z](http://doi.org/10.1016/0009-2614(94)01451-Z)
- (123) A.C. Reddy, D. Danovich, A. Ioffe, S. Shaik
“Electron Transfer Mechanistic Manifold and Variable Transition State Character. A Theoretical Investigation of Model Electron Transfer Processes between Nucleophiles and Ethane Cation Radicals”
J. Chem. Soc. Perkin Trans. 2, 1525-1539 (1995)
<http://doi.org/10.1039/P29950001525>
- (124) G.N. Sastry, S. Shaik
“Stereochemistry and Regiochemistry in Model Electron Transfer and Substitution Reactions of a Radical Anion with an Alkyl Halide”
J. Am. Chem. Soc., **117**, 3290-3291 (1995)
<http://doi.org/10.1021/Ja00116A041>
- (125) P.C. Hiberty, S. Humble, D. Danovich, S. Shaik
“What is Physically Wrong with the Description of Odd-Electron Bonding by Hartree-Fock Theory? A Simple Nonempirical Remedy”
J. Am. Chem. Soc., **117**, 9003-9011 (1995)
<http://doi.org/10.1021/Ja00140A017>

- (126) G. N. Sastry, A.C. Reddy, S. Shaik
 “Electron Transfer and Polar Reactions of Cyclizable Anion Radicals: Structural Consequences of Orbital Selection Rules and Chain-Length Constraints”
Angew. Chem., Int. Ed., **34**, 1495-1497 (1995)
<http://doi.org/10.1002/Anie.199514951>
Angew. Chem., **107**, 1619-1621 (1995).
- (127) S. Shaik, D. Danovich, A. Fiedler, D. Schröder, H. Schwarz
 “Two-State reactivity in Organometallic Gas-Phase Ion Chemistry”
Helv. Chim. Acta, **78**, 1393-1407 (1995)
<http://doi.org/10.1002/Hlca.19950780602>
- (128) A.C. Reddy, G.N. Sastry, S. Shaik
 “Electron Transfer Mechanisms: A Mechanistic Changeover Induced by an Intramolecular Spacer in a Model Reaction of the NH₃/ C₂H₄⁺ Pair”
J. Chem. Soc., Perkin Trans., **2**, 1717-1719 (1995)
<http://doi.org/10.1039/P29950001717>
- (129) S. Zilberg, Y. Haas, S. Shaik
 “Electronic Spectrum of Anthracene: an Ab-Initio Molecular Orbital Calculation Combined with a Valence Bond Interpretation”
J. Phys. Chem., **99**, 16558-16565 (1995)
<http://doi.org/10.1021/J100045A012>

1996

- (130) S. Shaik, A. Shurki, D. Danovich, P.C. Hiberty
 “Origins of the Exalted b_{2u} Frequency in the First Excited State of Benzene.”
J. Am. Chem. Soc., **118**, 666-671 (1996)
<http://doi.org/10.1021/Ja952376W>
- (131) G.N. Sastry, D. Danovich and S. Shaik
 “Towards the Definition of the Maximum Allowable Tightness of an Electron transfer Transition State in the Reactions of radical Anions and Alkyl Halides”
Angew. Chem., Int. Ed., **35**, 1098-1100 (1996)
<http://doi.org/10.1002/Anie.199610981>
Angew. Chem., **108**, 1208-1211 (1996).
- (132) S. Shaik, S. Zilberg, Y. Haas
 “A Kekulé-Crossing Model for the “Anomalous” behavior of the b_{2u} Modes of aromatic Hydrocarbons in the Lowest Excited 1B_{2u} State”
Acc. Chem. Res., **29**, 211-218 (1996)
<https://doi.org/10.1021/ar950206i>
- (133) D. Lauvergnant, P.C. Hiberty, D. Danovich, S. Shaik
 “Comparison of the C-Cl and Si-Cl Bonds. A Valence Bond Study”
J. Phys. Chem., **100**, 5715-5720 (1996)
<http://doi.org/10.1021/Jp960145L>
- (134) G.N. Sastry, S. Shaik
 “Structured Electron Transfer Transition State. Valence Bond Configuration Mixing Analysis and Ab Initio Calculations of the Reaction of Formaldehyde Radical Anion with Methyl Chloride”
J. Phys. Chem., **100**, 12241-12252 (1996)
<http://doi.org/10.1021/Jp952827Z>
- (135) E.M. Conwell, J. Perlstein, S. Shaik
 “Interchain Photoluminescence in Poly (phenylene vinylene) Derivatives”
Phys. Rev. B, **54**, part II, R2308-R2310 (1996)
<https://doi.org/10.1103/PhysRevB.54.R2308>
- (136) H. Zuilhof, J.P. Dinnocenzo, A.C. Reddy, S. Shaik
 “Comparative Study of Ethane and Propane Cation Radicals by B3LYP Density Functional and High-Level Ab Initio Methods”
J. Phys. Chem., **100**, 15774-15784 (1996)
<http://doi.org/10.1021/Jp961092A>

1997

- (137) L. Ebersson, R. González-Luque, M. Merchán, F. Radner, B.O. Roos, S. Shaik

- “Radical Cations of Non-alternant Systems as Probes of the Shaik-Pross VB Configuration Mixing Model”
J. Chem. Soc., Perkin Trans., 2, 463-472 (1997)
<http://doi.org/10.1039/A606702F>
- (138) D. Danovich, S. Shaik
 “Spin-Orbit Coupling in the Oxidative Activation of H-H by FeO⁺. Selection Rules and Reactivity Effects”
J. Am. Chem. Soc., **119**, 1773-1786 (1997)
<http://doi.org/10.1021/Ja963033G>
- (139) S. Shaik, A. Shurki, D. Danovich, P.C. Hiberty
 “A Different Story of Benzene”
J. Mol. Struct. (THEOCHEM), **398-399**, 155-167 (1997)
[http://doi.org/10.1016/S0166-1280\(96\)04934-2](http://doi.org/10.1016/S0166-1280(96)04934-2)
- (140) S. Shaik, D. Danovich, G.N. Sastry, P.Y. Ayala, H.B. Schlegel
 “Dissociative Electron Transfer, Substitution, and Borderline Mechanisms in Reactions of Ketyl Radical Anions. Differences and Difficulties in their Reaction Paths”
J. Am. Chem. Soc., **119**, 9237-9245 (1997)
<http://doi.org/10.1021/Ja971105D>
- (141) J.N. Harvey, D. Schröder, W. Koch, D. Danovich, S. Shaik, H. Schwarz
 “Electron-Transfer Reactivity in the Bond Activation of Organic Fluorides by Bare Metal Monocation”
Chem. Phys. Lett., **273**, 164-170 (1997)
[http://doi.org/10.1016/S0009-2614\(97\)01112-3](http://doi.org/10.1016/S0009-2614(97)01112-3)
- (142) J.N. Harvey, D. Schröder, W. Koch, D. Danovich, S. Shaik, H. Schwarz
 “Electron-Transfer Reactivity in the Bond Activation of Organic Fluorides by Bare Metal Monocation”
Chem. Phys. Lett., **278**, 391-397 (1997), *Erratum in Full*
- (143) A. Shurki, S. Shaik
 “The Distortive Tendency of Benzene π -Electrons: How is it related to structural Observables?”
Angew. Chem., Int. Ed., **36**, 2205-2208 (1997)
<https://doi.org/10.1002/anie.199722051>
Angew. Chem., **109**, 2322-2324 (1997).

1998

- (144) G.N. Sastry, S. Shaik
 “Mechanistic Crossover Induced by Steric Hindrance: A Theoretical Study of Electron Transfer and Substitution Mechanisms of Cyanoformaldehyde Anion Radical and Alkyl Halides”
J. Am. Chem. Soc., **120**, 2131-2145 (1998)
<http://doi.org/10.1021/Ja972746B>
- (145) S. Shaik, M. Filatov, D. Schröder, H. Schwarz
 “Electronic Structure Makes a Difference: Cytochrome P-450 Mediated Hydroxylation of Hydrocarbons as a Two-State Reactivity Paradigm”
Chem. Eur. J., **4**, 193-199 (1998)
[http://doi.org/10.1002/\(Sici\)1521-3765\(19980210\)4:2%3C193::Aid-Chem193%3E3.0.Co;2-Q](http://doi.org/10.1002/(Sici)1521-3765(19980210)4:2%3C193::Aid-Chem193%3E3.0.Co;2-Q)
- (146) REVIEW
 S. Shaik
 “The Valence Bond Curve Crossing Model for Chemical Reactivity: An Interface between Computational Chemistry, Theory and Experiment”
Encyclopedia of Computational Chemistry, **5**, 3143-3156 (1998)
 P.v.R. Schleyer, H.F. Schaefer, P.R. Schreiner, Eds., Wiley & Sons.
- (147) D. Danovich, C.M. Marian, T. Neuheuser, S.D. Peyerimhoff, S. Shaik
 “Spin-Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C₂H₄: A Quantitative Study and Qualitative Analysis”
J. Phys. Chem. A, **102**, 5923-5936 (1998)
<http://doi.org/10.1021/Jp980391S>
- (148) A. Shurki, S. Shaik
 “The Perfectly Resonating State: A Chemical Model for the Transition State.”
J. Mol. Struct. (THEOCHEM), **424**, 37-45 (1998)
[http://doi.org/10.1016/S0166-1280\(97\)00223-6](http://doi.org/10.1016/S0166-1280(97)00223-6)
 The Lionel Salem Festschrift Issue
- (149) J.P. Dinnocenzo, M. Merchán, B.O. Roos, S. Shaik, H. Zuilhof
 “Electronic Spectra of Phenylcyclopropane and Cumene Cation Radicals: Interplay of Experiment and Theory”

- J. Phys. Chem. A*, **102**, 8979-8987 (1998)
<http://doi.org/10.1021/Jp9820673>
- (150) M. Filatov, S. Shaik
 “Theoretical Investigation of Two-State-Reactivity Pathways of H-H Activation by FeO⁺: Addition-Elimination, “Rebound” and Oxene-Insertion Mechanisms”
J. Phys. Chem. A, **102**, 3835-3846 (1998)
<http://doi.org/10.1021/Jp980929U>
- (151) S. Grimme, M. Woeller, S.D. Peyerimhoff, D. Danovich, S. Shaik
 “Theoretical Study of the Radiationless Decay Channels of Triplet State Norbornene”
Chem Phys. Lett., **287** 601-607 (1998)
[http://doi.org/10.1016/S0009-2614\(98\)00179-1](http://doi.org/10.1016/S0009-2614(98)00179-1)
- (152) S. Zilberg, Y. Haas, D. Danovich, S. Shaik
 “The Twin-Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibullvalene Rearrangement”
Angew Chem., Int. Ed., **37**, 1394-1397 (1998)
[http://doi.org/10.1002/\(SICI\)1521-3773\(19980605\)37:10%3C1394::AID-ANIE1394%3E3.0.CO;2-J](http://doi.org/10.1002/(SICI)1521-3773(19980605)37:10%3C1394::AID-ANIE1394%3E3.0.CO;2-J)
Angew. Chem., **110**, 1470-1473 (1998).
- (153) M. Filatov, S. Shaik
 “Spin-Restricted Density Functional Approach to Open-Shell Problem”
Chem. Phys. Lett., **288**, 689-697 (1998)
[http://doi.org/10.1016/S0009-2614\(98\)00364-9](http://doi.org/10.1016/S0009-2614(98)00364-9)
- (154) W. Wu, S.-J. Zhong, S. Shaik
 “VBDFT(s): A Huckel-type Semi-empirical Valence Bond Method Scaled to Density Functional Energies. Application to Linear Polyenes”
Chem. Phys. Lett., **292**, 7-14 (1998)
[http://doi.org/10.1016/S0009-2614\(98\)00684-8](http://doi.org/10.1016/S0009-2614(98)00684-8)

1999

- (155) S. Shaik, A. Shurki
 “Valence Bond Diagrams and Chemical Reactivity”
Angew. Chem., Int. Ed., **38**, 586-625 (1999).
[https://doi.org/10.1002/\(SICI\)1521-3773\(19990301\)38:5<586::AID-ANIE586>3.0.CO;2-T](https://doi.org/10.1002/(SICI)1521-3773(19990301)38:5<586::AID-ANIE586>3.0.CO;2-T)
Angew. Chem. **111**, 616-657 (1999).
- (156) D. Danovich, W. Wu, S. Shaik
 “No-Pair Bonding in the High-Spin ³Σ_u⁺ State of Li₂. A Valence Bond Study of its Origins”
J. Am. Chem. Soc., **121**, 3165-3174 (1999)
<http://doi.org/10.1021/Ja982913N>
- (157) A. Shurki, P.C. Hiberty, S. Shaik
 “Charge-Shift Bonding in Group IVB Halides: A Valence Bond Study of MH₃-Cl (M = C, Si, Ge, Sn, Pb) Molecules” *J. Am. Chem. Soc.*, **121**, 822-834 (1999)
<http://doi.org/10.1021/Ja995530D>
- (158) A. Shurki, P.C. Hiberty, S. Shaik
J. Am. Chem. Soc., **121**, 9768 (1999) (Errata).
<https://doi.org/10.1021/ja995530d>
- (159) M. Filatov, N. Harris, S. Shaik
 “A Theoretical Study of Electronic Factors Affecting Hydroxylation by Model Ferryl Complexes of Cytochrome P-450 and Horseradish Peroxidase”
J. Chem. Soc., Perkin Trans., 2, 399-410 (1999)
<http://doi.org/10.1039/A809385G>
- (160) M. Filatov, S. Shaik
 “Application of Spin-Restricted Open-Shell Kohn-Sham Method to Atomic and Molecular Multiplet States”
J. Chem. Phys., **110**, 116-125 (1999)
<http://doi.org/10.1063/1.477941>
- (161) N. Harris, W. Wu, W.H. Saunders, Jr., S. Shaik
 “Origins of Non-perfect Synchronization in the Lowest Energy Path of the Identity Proton Transfer Reaction of Allyl Anion + Propene: A VBSCF Study”
J. Phys. Org. Chem., **12**, 259-262 (1999)
[http://doi.org/10.1002/\(SICI\)1099-1395\(199903\)12:3%3C259::Aid-Poc153%3E3.0.Co;2-H](http://doi.org/10.1002/(SICI)1099-1395(199903)12:3%3C259::Aid-Poc153%3E3.0.Co;2-H)

- (162) W. Wu, S. Shaik
 “VB-DFT: A Nonempirical Hybrid method Combining Valence Bond Theory and Density Functional Energies”
Chem. Phys. Lett., **301**, 37-42 (1999)
[http://doi.org/10.1016/S0009-2614\(99\)00011-1](http://doi.org/10.1016/S0009-2614(99)00011-1)
- (163) M. Filatov, S. Shaik
 “A Spin-Restricted Ensemble-Referenced Kohn-Sham Method and Its Application to Diradicaloid Situations”
Chem. Phys. Lett., **304**, 429-437 (1999)
[http://doi.org/10.1016/S0009-2614\(99\)00336-X](http://doi.org/10.1016/S0009-2614(99)00336-X)
- (164) M. Filatov, S. Shaik
 “Tetramethyleneethane (TME) Diradical: Experiment and Density Functional Theory Reach and Agreement”
J. Phys. Chem. A, **103**, 8885-8889 (1999)
<http://doi.org/10.1021/Jp9920489>
- (165) N. Harris, S. Shaik, D. Schröder, H. Schwarz
 “Single- and Two-State Reactivity in the Gas Phase C-H Bond Activation of Norbornane by ‘Bare’ FeO⁺”
Helv. Chem. Acta, **82**, 1784-1797 (1999)
[http://doi.org/10.1002/\(Sici\)1522-2675\(19991006\)82:10%3C1784::Aid-Hlca1784%3E3.0.Co:2-M](http://doi.org/10.1002/(Sici)1522-2675(19991006)82:10%3C1784::Aid-Hlca1784%3E3.0.Co:2-M)
- (166) M. Filatov, N. Harris, S. Shaik
 “On the ‘Rebound’ Mechanism of Alkane Hydroxylation by Cytochrome P450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step”
Angew. Chem., Int. Ed., **38**, 3510-3512 (1999)
[http://doi.org/10.1002/\(Sici\)1521-3773\(19991203\)38:23%3C3510::Aid-Anie3510%3E3.0.Co:2-#](http://doi.org/10.1002/(Sici)1521-3773(19991203)38:23%3C3510::Aid-Anie3510%3E3.0.Co:2-#)
Angew. Chem. **111**, 3730-3733 (1999)

2000

- (167) J.M. Galbraith, A. Shurki, S. Shaik
 “A Valence Bond Study of the Bonding in First Row Transition Metal Hydride Cations: What Energetic Role Does Covalency Play?”
J. Chem. Phys. A, **104**, 1262-1270 (2000)
<http://doi.org/10.1021/Jp9924878>
- (168) M. Woeller, S. Grimme, S.D. Peyerimhoff, D. Danovich, M. Filatov, S. Shaik
 “A Theoretical Study of the Radiationless Decay Mechanisms of Cyclic Alkenes in the Lowest Triplet State”
J. Phys. Chem. A, **104**, 5366-5373 (2000)
<http://doi.org/10.1021/Jp0003398>
- (169) J.M. Galbraith, E. Blank, S. Shaik, P.C. Hiberty
 “ π Bonding in second and Third Row Molecules: Testing the Strength of Linus’s Blanket”
Chem. Eur. J., **6**, 2425-2434 (2000)
[http://doi.org/10.1002/1521-3765\(20000703\)6:13%3C2425::Aid-Chem2425%3E3.0.Co:2-0](http://doi.org/10.1002/1521-3765(20000703)6:13%3C2425::Aid-Chem2425%3E3.0.Co:2-0)
- (170) M. Filatov, S. Shaik, M. Woeller, S. Grimme, S.D. Peyerimhoff
 “Locked Alkenes with a Short Triplet State’s Lifetime”
Chem. Phys. Lett., **316**, 135-140 (2000)
[http://doi.org/10.1016/S0009-2614\(99\)00965-3](http://doi.org/10.1016/S0009-2614(99)00965-3)
- (171) J.M. Galbraith, P.R. Schreiner, N. Harris, W. Wu, A. Wittkopp, S. Shaik
 “A Valence Bond Study of the Bergman Cyclization: Geometric Features, Resonance Energy, and Nucleus-Independent Chemical Shift (NICS) Values”
Chem. Eur. J., **6**, 1446-1454 (2000)
[https://doi.org/10.1002/\(SICI\)1521-3765\(20000417\)6:8%3C1446::AID-CHEM1446%3E3.0.CO:2-I](https://doi.org/10.1002/(SICI)1521-3765(20000417)6:8%3C1446::AID-CHEM1446%3E3.0.CO:2-I)
- (172) N. Harris, S. Cohen, M. Filatov, F. Ogliaro, S. Shaik
 “Two-State Reactivity in the Rebound Step of Alkane Hydroxylation by Cytochrome P-450. Origins of Free Radicals with Finite Lifetimes”
Angew. Chem., Int. Ed., **39**, 2003-2007 (2000)
[https://doi.org/10.1002/1521-3773\(20000602\)39:11%3C2003::AID-ANIE2003%3E3.0.CO:2-M](https://doi.org/10.1002/1521-3773(20000602)39:11%3C2003::AID-ANIE2003%3E3.0.CO:2-M)
- (173) CHAPTER
 D. Schröder, S. Shaik, H. Schwarz
 “Characterization, Orbital Description, and Reactivity Patterns of Transition-Metal Oxo Species in the Gas Phase”, in: “Metal-oxo and Metal-peroxo Species in Catalytic Oxidations”, B. Meunier, Editor
Struct. Bonding, **97**, 92-123 (2000)
- (174) D. Schröder, S. Shaik, H. Schwarz,
 “Two-State Reactivity as a new Concept in Organometallic Chemistry”

- Acc. Chem. Res.*, **33**, 139-145 (2000)
<https://doi.org/10.1021/ar990028j>
- (175) W. Wu, D. Danovich, A. Shurki, S. Shaik
 “Using Valence Bond Theory to Understand Electronic Excited States: Application to the Hidden Excited State (2^1A_g) of $C_{2n}H_{2n+2}$ ($n = 2-14$) Polyenes”
J. Phys. Chem. A, **104**, 8744-8758 (2000)
<https://doi.org/10.1021/jp000847h>
- (176) M. Filatov, S. Shaik
 “Diradicaloids: Description by the Spin-Restricted, Ensemble-Referenced Kohn-Sham Density Functional Method”
J. Phys. Chem. A, **104**, 6628-6636 (2000)
<https://doi.org/10.1021/jp0002289>
- (177) J.N. Harvey, S. Grimme, M. Woeller, S.D. Peyerimhoff, D. Danovich, S. Shaik
 “Computational Prediction of the ISC Rate for Triplet Norbornene”
Chem. Phys. Lett., **322**, 358-362 (2000)
[https://doi.org/10.1016/S0009-2614\(00\)00442-5](https://doi.org/10.1016/S0009-2614(00)00442-5)
- (178) F. Ogliaro, N. Harris, S. Cohen, M. Filatov, S.P. de Visser, S. Shaik
 “A Model ‘Rebound’ Mechanism of Hydroxylation by Cytochrome P450: Stepwise and Effectively Concerted Pathways, and their Reactivity Patterns”
J. Am. Chem. Soc., **122**, 8977-8989 (2000)
<https://doi.org/10.1021/ja991878x>
- (179) N. Harris, W. Wu, W.H. Saunders, Jr., S. Shaik
 “Origins of Nonperfect Synchronization in the Lowest-Energy Path of Identity Proton Transfer reactions leading to Delocalized Anions: A VBSCF Study”
J. Am. Chem. Soc., **122**, 6754-6758 (2000)
<https://doi.org/10.1021/ja001032p>
- (180) M. Filatov, W. Reickien, S.D. Peyerimhoff, S. Shaik
 “What are the Reasons for the Kinetic Stability of a Mixture of H_2 and O_2 ?”
J. Phys. Chem. A, **104**, 12014-12020 (2000)
<https://doi.org/10.1021/jp0032208>
- (181) F. Ogliaro, S. Cohen, M. Filatov, N. Harris, S. Shaik
 “The High-valent Compound of Cytochrome P450: The Nature of the Fe-S Bond and the Role of the Thiolate Ligand as an Internal Electron Donor”
Angew. Chem., Int. Ed., **39**, 3851-3855 (2000)
[https://doi.org/10.1002/1521-3773\(20001103\)39:21%3C3851::AID-ANIE3851%3E3.0.CO;2-9](https://doi.org/10.1002/1521-3773(20001103)39:21%3C3851::AID-ANIE3851%3E3.0.CO;2-9)
Angew. Chem., **122**, 4009-4013 (2000).
 Erratum: *Angew. Chem., Int. Ed.*, **40**, 647 (2001).
- (182) F. Ogliaro, M. Filatov, S. Shaik
 “Alkane Hydroxylation by Cytochrome P450: Is Kinetic Isotope Effect a Reliable Probe of Transition State Structure?”
Eur. J. Inorg. Chem., 2455-2458 (2000)
[https://doi.org/10.1002/1099-0682\(200012\)2000:12%3C2455::AID-EJIC2455%3E3.0.CO;2-4](https://doi.org/10.1002/1099-0682(200012)2000:12%3C2455::AID-EJIC2455%3E3.0.CO;2-4)
- (183) F. Ogliaro, S. Cohen, S.P. de Visser, S. Shaik
 “Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450: What Kind of a Radical Is It Really?”
J. Am. Chem. Soc., **122**, 12892-12893 (2000)
<https://doi.org/10.1021/ja005619f>
- (184) S.P. de Visser, Y. Alpert, D. Danovich, S. Shaik
 “No-Pair Bonding in High-Spin Lithium Clusters: n^+Li_n ($n=2-6$)”
J. Phys. Chem. A, **104**, 11223-11231 (2000)
<https://doi.org/10.1021/jp002723a>
- (185) M. Filatov, S. Shaik
 “Artificial Symmetry Breaking in Radicals Is Avoided by the Use of the Ensemble-reference Kohn-Sham (REKS) Method”
Chem. Phys. Lett., **332**, 409-419 (2000)
[https://doi.org/10.1016/S0009-2614\(00\)01257-4](https://doi.org/10.1016/S0009-2614(00)01257-4)
- (186) S.P. de Visser, M. Filatov, S. Shaik
 “REKS Calculations on *ortho*- *meta*- and *para*-Benzyne”
Phys. Chem. Chem. Phys., **2**, 5046-5048 (2000)

- <https://doi.org/10.1039/B006786P>
 (187) D. Schröder, C. Trage, H. Schwarz, D. Danovich, S. Shaik
 “Inner-Sphere Electron Transfer in Metal-Cation Chemistry”
Int. J. Mass Spectrom., **200**, 163-175 (2000)
[https://doi.org/10.1016/S1387-3806\(00\)00349-3](https://doi.org/10.1016/S1387-3806(00)00349-3)

2001

- (188) D. Danovich, F. Ogliaro, M. Karni, Y. Apeloig, D.L. Cooper, S. Shaik
 “Silynes (RC≡SiR') and Disilynes (RSi≡SiR'): Why Are Less Bonds Worth Energetically More?”
Angew. Chem., Int. Ed., **40**, 4023-4026 (2001); **40**, 647(2001) (Erratum)
[https://doi.org/10.1002/1521-3773\(20011105\)40:21%3C4023::AID-ANIE4023%3E3.0.CO;2-Z](https://doi.org/10.1002/1521-3773(20011105)40:21%3C4023::AID-ANIE4023%3E3.0.CO;2-Z)
- (189) V. Bakken, D. Danovich, S. Shaik, H.B. Schlegel
 “A Single Transition State Serves two Mechanisms: An Ab Initio Classical Trajectory Study of the Electron Transfer and Substitution Mechanisms in Reactions of Ketyl Radical Anions with Alkyl Halides”
J. Am. Chem. Soc., **123**, 130-134 (2001)
<https://doi.org/10.1021/ja002799k>
- (190) S. Shaik, A. Shurki, D. Danovich, P.C. Hiberty
 “A Different Story of π -Delocalization- The Distortivity of π -Electrons and Its Chemical Manifestations”
Chem. Rev., **101**, 1501-1540 (2001).
<https://doi.org/10.1021/cr990363l>
- (191) S. Shaik, W. Wu, K. Dong, L. Song, P.C. Hiberty
 “Identity Hydrogen Abstraction Reactions, $X\cdot + H-X' \rightarrow X-H + X'\cdot$ ($X=X'=CH_3, SiH_3, GeH_3, SnH_3, PbH_3$): A Valence Bond Modeling”
J. Phys. Chem. A, **105**, 8226-8235 (2001)
<https://doi.org/10.1021/jp011251c>
- (192) K. Jug, P.C. Hiberty, S. Shaik
 “ σ - π Energy Separation in Modern Electronic Theory for Ground State Conjugated Systems”
Chem. Rev., **101**, 1477-1500 (2001)
<https://doi.org/10.1021/cr990328e>
- (193) S.P. de Visser, F. Ogliaro, N. Harris, S. Shaik
 “Multi-State Epoxidation of Ethene by Cytochrome P450: a Quantum Chemical Study”
J. Am. Chem. Soc., **123**, 3037-3047 (2001)
<https://doi.org/10.1021/ja003544+>
- (194) S.P. de Visser, F. Ogliaro, S. Shaik
 “How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study”
Angew. Chem. Int. Ed., **40**, 2871-2874 (2001)
[https://doi.org/10.1002/1521-3773\(20010803\)40:15%3C2871::AID-ANIE2871%3E3.0.CO;2-R](https://doi.org/10.1002/1521-3773(20010803)40:15%3C2871::AID-ANIE2871%3E3.0.CO;2-R)
- (195) S.P. de Visser, M. Filatov, S. Shaik
 “Myers-Saito and Schmittel Cyclization of hepta-1,2,4-triene-6-yne: a Theoretical REKS Study”
Phys. Chem. Chem. Phys., **3**, 1242-1245 (2001)
<https://doi.org/10.1039/B009965L>
- (196) F. Ogliaro, S.P. de Visser, J.T. Groves, S. Shaik
 “Chameleon States: The High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analog”
Angew. Chem., Int. Ed., **40**, 2874-2878 (2001)
[https://doi.org/10.1002/1521-3773\(20010803\)40:15%3C2874::aid-anie2874%3E3.0.co;2-9](https://doi.org/10.1002/1521-3773(20010803)40:15%3C2874::aid-anie2874%3E3.0.co;2-9)
- (197) F. Ogliaro, S.P. de Visser, J.T. Groves, S. Shaik
 Corrigendum: “Chameleon States: The High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analog”
Angew. Chem., Int. Ed., **40**, 3503 (2001)
[https://doi.org/10.1002/1521-3773\(20011001\)40:19%3C3503::AID-ANIE33333503%3E3.0.CO;2-O](https://doi.org/10.1002/1521-3773(20011001)40:19%3C3503::AID-ANIE33333503%3E3.0.CO;2-O)
- (198) S. Shaik
 “Chemical Reactivity and Valence Bond Diagrams: A Personal Account”
Chem. Isr., **6**, 4-11 (2001).
- (199) W. Wu, Y. Luo, L. Song, S. Shaik
 “VBDFT(s)- a Semiempirical Valence Bond Method: Application to Linear Polyenes Containing Oxygen and Nitrogen Heteroatoms”
Phys. Chem. Chem. Phys., **3**, 5459-5465 (2001)

- <http://dx.doi.org/10.1039/b107505e>
- (200) F. Ogliaro, S.P. de Visser, S. Cohen, J. Kaneti, S. Shaik
 “The Experimentally Elusive Oxidant of Cytochrome P450: A Theoretical ‘Trapping’ Defining more Closely the ‘Real’ Species”
ChemBioChem, **2**, 848-851 (2001)
[https://doi.org/10.1002/1439-7633\(20011105\)2:11%3C848::AID-CBIC848%3E3.0.CO;2-0](https://doi.org/10.1002/1439-7633(20011105)2:11%3C848::AID-CBIC848%3E3.0.CO;2-0)
- (201) S.P. de Visser, F. Ogliaro, Z. Gross, S. Shaik
 “What is the Difference between the Manganese Porphyrin and Corrole Analogs of Cytochrome P450’s Compound I?”
Chem. Eur. J., **7**, 4954-4960 (2001)
[https://doi.org/10.1002/1521-3765\(20011119\)7:22%3C4954::AID-CHEM4954%3E3.0.CO;2-U](https://doi.org/10.1002/1521-3765(20011119)7:22%3C4954::AID-CHEM4954%3E3.0.CO;2-U)
- (202) S. Cohen, F. Ogliaro, S.P. de Visser, J. Kaneti, S. Shaik
 “Does Polarizing Medium Affect the Kinetics of Alkane Hydroxylation by Compound I of Cytochrome P450?”
J. Inorg. Biochem., **86**, 183 (2001)
- (203) S.P. de Visser, F. Ogliaro, S. Shaik
 “Does Stereospecific Oxidation by Compound I of Cytochrome P450 Ever Proceed in a Concerted Manner?”
J. Inorg. Biochem., **86**, 198 (2001)
- (204) F. Ogliaro, S.P. de Visser, S. Shaik
 “Does the Catalytic Cycle of Cytochrome P450 Involve a Second Oxidant? A Theoretical Investigation of the hydroperoxo Hypothesis”
J. Inorg. Biochem., **86**, 363 (2001)

2002

- (205) W. Wu, S. Shaik, W.H. Saunders, Jr.
 “Comparative Study of Identity Proton-Transfer Reactions between Simple Atoms and Groups by VB Methods”
J. Phys. Chem. A, **106**, 11616-11622 (2002)
<https://doi.org/10.1021/jp021452w>
- (206) CHAPTER
 P.C. Hiberty, S. Shaik
 “BOVB- A Valence Bond Method Incorporating Static and Dynamic Correlation Effects”
Theoretical and Computational Chemistry Vol 10, in: “Valence Bond Theory”
 D.L. Cooper, D.J. Klein, Eds. Elsevier Publications, NY, 2002, *Chapter 7*, pp 187-225
- (207) L. Song, W. Wu, K. Dong, P.C. Hiberty, S. Shaik
 “Valence Bond Modeling of Barriers in the Nonidentity Hydrogen Abstraction Reactions,
 $X^{\bullet} + H-X \rightarrow X^{\prime}-H + X^{\bullet}$ ($X \neq X^{\prime} = CH_3, SiH_3, GeH_3, SnH_3, PbH_3$)”
J. Phys. Chem. A, **106**, 11361-11370 (2002)
<https://doi.org/10.1021/jp026438y>
- (208) S. P. de Visser, D. Danovich, W. Wu, S. Shaik
 “Ferromagnetic Bonding: Properties of High-Spin Lithium Clusters; $^{n+1}Li_n$ ($n = 2-12$)”
J. Phys. Chem. A, **106**, 4961-4969 (2002)
<https://doi.org/10.1021/jp014665e>
- (209) S.P. de Visser, F. Ogliaro, S. Shaik
 “Stereospecific Epoxidation by Compound I of Cytochrome P450 does not proceed in a Concerted Synchronous Manner”
J. Chem. Soc., Chem. Commun., 2322-2323 (2002)
<https://doi.org/10.1039/B105571M>
- (210) P.C. Hiberty, S. Shaik
 “Breathing-Orbital Valence Bond Method- A Modern Valence Bond method that Includes Dynamic Correlation”
Theor. Chem. Acc., **108**, 255-275 (2002)
<https://doi.org/10.1007/s00214-002-0364-8>
- (211) F. Ogliaro, S.P. de Visser, S. Cohen, P.K. Sharma, S. Shaik
 “Searching for the Second oxidant in the Catalytic Cycle of Cytochrome P450: A Theoretical Investigation of the Iron(III)-Hydroperoxo Species and Its Epoxidation Pathways”
J. Am. Chem. Soc., **124**, 2806-2817 (2002)
<https://doi.org/10.1021/ja0171963>
- (212) S.P. de Visser, F. Ogliaro, P.K. Sharma, S. Shaik
 “Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I”

- Angew. Chem., Int. Ed.*, **41**, 1947-1951 (2002)
[https://doi.org/10.1002/1521-3773\(20020603\)41:11%3C1947::AID-ANIE1947%3E3.0.CO;2-W](https://doi.org/10.1002/1521-3773(20020603)41:11%3C1947::AID-ANIE1947%3E3.0.CO;2-W)
- (213) W. Wu, L. Song, Z. Cao, Q. Zhang, S. Shaik
 “Valence Bond Configuration Interaction: A Practical ab initio Valence Bond Method that Incorporates Dynamic Correlation”
J. Phys. Chem. A, **106**, 2721-2726 (2002)
<https://doi.org/10.1021/jp0141272>
- (214) F. Ogliaro, S.P. de Visser, S. Shaik
 “The ‘Push’ Effect of the Thiolate Ligands in Cytochrome P450: A Theoretical Gauging”
J. Inorg. Biochem., **91**, 554-567 (2002)
[https://doi.org/10.1016/s0162-0134\(02\)00437-3](https://doi.org/10.1016/s0162-0134(02)00437-3)
- (215) S. Shaik, S.P. de Visser, W. Wu, L. Song, P.C. Hiberty
 “Reply to Comment on: “Identity Hydrogen Abstraction Reactions, $X\cdot + H-X' \rightarrow X-H + X'\cdot$ ($X=X' \square CH_3, SiH_3, GeH_3, SnH_3, PbH_3$): A Valence Bond Modeling”
J. Phys. Chem. A, **106**, 5043-5045 (2002)
<https://doi.org/10.1021/jp015589i>
- (216) J.C. Schöneboom, H. Lin, N. Reuter, W. Thiel, S. Cohen, F. Ogliaro, S. Shaik
 “The Elusive Oxidant of Cytochrome P450 Enzymes: Characterization by Combined Quantum Mechanical/Molecular Mechanical (QM/MM) Calculations”
J. Am. Chem. Soc., **124**, 8142-8151 (2002)
<https://doi.org/10.1021/ja026279w>
- (217) D. Cremer, M. Filatov, V. Polo, E. Kraka, S. Shaik
 “Implicit and Explicit Coverage of Multi-reference Effect by Density Functional Theory”
J. Mol. Sci., **3**, 604-638 (2002)
<https://doi.org/10.3390/i3060604>
 (an electronic journal <http://www.mdpi.org/ijms/>)
- (218) S.P. de Visser, F. Ogliaro, P.K. Sharma, S. Shaik
 “What Factors Affect the Regioselectivity of Oxidation by Cytochrome P450? A DFT Study of Allylic Hydroxylation and Double Bond Epoxidation in a Model Reaction”
J. Am. Chem. Soc., **124**, 11809-11826 (2002)
<https://doi.org/10.1021/ja026872d>
- (219) S. Shaik, S.P. de Visser, F. Ogliaro, H. Schwarz, D. Schröder
 “Two-State Reactivity Mechanism of Hydroxylation and Epoxidation by Cytochrome P-450 Revealed by Theory”
Curr. Opin. Chem. Biol., **6**, 556-567 (2002)
[https://doi.org/10.1016/s1367-5931\(02\)00363-0](https://doi.org/10.1016/s1367-5931(02)00363-0)
- (220) S.P. de Visser, D. Danovich, S. Shaik
 “Ferromagnetic Bonding in High-Spin Alkali-Metal Clusters. How Does Sodium Compare to Lithium?”
Phys. Chem. Chem. Phys., **5**, 158-164 (2002)
<https://doi.org/10.1039/B207155J>

2003

- (221) A. Shurki, P.C. Hiberty, F. Dijkstra, S. Shaik
 “Aromaticity and Antiaromaticity: What Role do Ionic Configurations Play in Delocalization and Induction of Magnetic Properties?”
J. Phys. Org. Chem., **16**, 731-745 (2003)
<https://doi.org/10.1002/poc.658>
- (222) S.P. de Visser, J. Kaneti, R. Neumann, S. Shaik
 “Fluorinated Alcohols Enable Olefin Epoxidation by H_2O_2 : Template Catalysis”
J. Org. Chem., **68**, 2903-2912 (2003)
<https://doi.org/10.1021/jo034087t>
- (223) S. Shaik, P.C. Hiberty
 “Myth and Reality in the Attitude toward Valence-Bond (VB) Theory: Are Its ‘Failures’ Real?”
Helv. Chim. Acta, **86**, 1063-1084 (2003)
<https://doi.org/10.1002/hlca.200390094>
- (224) S. Shaik
 “Chemistry- A Central Pillar of Human Culture”
Angew. Chem., Int. Ed., **42**, 3208-3215 (2003)

- <https://doi.org/10.1002/anie.200330038>
- (225) S. Shaik
 “Die Chemie - eine zentrale Saule der menschlichen Kultur”
Angew. Chem., **115**, 3326-3333 (2003).
<https://doi.org/10.1002/ange.200230038>
- (226) S.P. de Visser, M. Filatov, P.R. Schreiner, S. Shaik
 “A REKS Assessment of the Face-Diagonal Bond in 1,3-Dihydrocubane and a Comparison with Benzyne Radicals”
Eur. J. Org. Chem., 2003, 4199-4204 (2003)
<https://doi.org/10.1002/ejoc.200300201>
- (227) P.K. Sharma, S.P. de Visser, F. Ogliaro, S. Shaik
 “Is the Ruthenium Analog of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction”
J. Am. Chem. Soc., **125**, 2291-2300 (2003)
<https://doi.org/10.1021/ja0282487>
- (228) P.K. Sharma, S.P. de Visser, S. Shaik
 “Can a Single Oxidant with Two Spin-States Masquerade as Two different Oxidants? A Study of the Sulfoxidation Mechanism by Cytochrome P450”
J. Am. Chem. Soc., **125**, 8698-8699 (2003)
<https://doi.org/10.1021/ja035135u>
- (229) L. Song, W. Wu, P.C. Hiberty, D. Danovich, S. Shaik
 “An Accurate Barrier for the Hydrogen Exchange Reaction from Valence Bond Theory: Is this Coming of Age?”
Chem. Eur. J., **9**, 4540-4547 (2003)
<https://doi.org/10.1002/chem.200305093>
- (230) S.P. de Visser, S. Shaik
 “A Proton-Shuttle Mechanism Mediated by the Porphyrin in Benzene Hydroxylation by Cytochrome P450 Enzymes”
J. Am. Chem. Soc., **125**, 7413-7424 (2003)
<https://doi.org/10.1021/ja034142f>
- (231) R. Ben-Daniel, S.P. de Visser, S. Shaik, R. Neumann
 “Electrophilic Aromatic Chlorination and Haloperoxidation of Chloride Catalyzed by Polyfluorinated Alcohols: A New Manifestation of Template Catalysis”
J. Am. Chem. Soc., **125**, 12116-12117 (2003)
<https://doi.org/10.1021/ja0364524>
- (232) S.P. de Visser, S. Shaik, P.K. Sharma, D. Kumar, W. Thiel
 “The Active Species of Horseradish Peroxidase (HRP) and Cytochrome P450: Two Electronic Chameleons”
J. Am. Chem. Soc. **125**, 15779-15788 (2003)
<https://doi.org/10.1021/ja0380906>
- (233) P.K. Sharma, S. Shaik
 “Science: Viewing La Vega” (Web site review)
Angew. Chem., Int. Ed., **42**, 968-969 (2003)
- (234) R. Hoffmann, S. Shaik, P.C. Hiberty
 “A Conversation on VB vs. MO Theory: A Never Ending Rivalry?”
Acc. Chem. Res., **36**, 750-756 (2003)
<https://doi.org/10.1021/ar030162a>
- (235) S. Shaik
 “The Protein, the Active Species, and the Chameleon: Reactivity Patterns of Oxygen Transfer by P450”
Proceedings of the 13th International Conference on Cytochrome P450, Prague, June 29-July 3, 2003, P. Anzenbacher, J. Hudecek, Eds. Monduzzi Editore, Bologna, Italy, 2003, pp 93-97.
- (236) D. Kumar, S.P. de Visser, S. Shaik
 “How Does Product Isotope Effect Prove the Operation of a Two-State ‘Rebound’ Mechanisms in C-H Hydroxylation by Cytochrome P450?”
J. Am. Chem. Soc., **125**, 13024-13025 (2003)
<https://doi.org/10.1021/ja036906x>

2004

- (237) P.C. Hiberty, S. Shaik

- “The Distortive Tendencies of π -Electronic Systems, the Relationship to Isoelectronic σ -Bonded Analogs, and Observables: A Description Free of the Classical Paradoxes”
Phys. Chem. Chem. Phys., **6**, 224-231 (2004)
<https://doi.org/10.1039/B310496F>
- (238) S.P. de Visser, D. Kumar, S. Shaik
 “How Do Aldehyde Side Products Occur During Alkene Epoxidation by Cytochrome P450? Theory Reveals a State-Specific Multi-State Scenario where the High-Spin Component leads to all Side Products”
J. Inorg. Biochem., **98**, 1183-1193 (2004)
<https://doi.org/10.1016/j.jinorgbio.2004.01.015>
- (239) Y. Luo, L. Song, W. Wu, D. Danovich, S. Shaik
 “The Ground and Excited States of Polyenyl Radicals, $C_{2n-1}H_{2n+1}$ ($n = 2-13$): A Valence Bond Study”
ChemPhysChem, **5**, 515-528 (2004)
<https://doi.org/10.1002/cphc.200300935>
- (240) S.P. de Visser, P.K. Sharma, D. Kumar, R. Neuman, S. Shaik
 “Computer Generated High-Valent Iron-Oxo and manganese-Oxo Species with Polyoxometalate Ligands: How do they compare with the Iron-Oxo Species of Heme Enzymes?”
Angew. Chem., Int. Ed., **43**, 5661-5665 (2004)
<https://doi.org/10.1002/anie.200453867>
- (241) J.C. Schöneboom, S. Cohen, H. Lin, S. Shaik, W. Thiel
 “Quantum Mechanical/Molecular Mechanical Investigation of the Mechanism of C-H Hydroxylation of Camphor by Cytochrome P450_{cam}: Theory Supports a Two-State Rebound Mechanism”
J. Am. Chem. Soc., **126**, 4017-4034 (2004).
<https://doi.org/10.1021/ja039847w>
- (242) J. Li, X. Li, S. Shaik, H.B. Schlegel
 “Single Transition State Serves Two Mechanisms. Ab Initio Classical Trajectory Calculations of the Substitution-Electron Transfer Branching Ratio of $CH_2O\cdot + CH_3Cl$ ”
J. Phys. Chem. A, **108**, 8526-8532 (2004)
<https://doi.org/10.1021/jp046827n>
- (243) S. Shaik, S. Cohen, S.P. de Visser, P.K. Sharma, D. Kumar, S. Kozuch, F. Ogliaro, D. Danovich
 “The “Rebound Controversy”: An Overview and Theoretical Modeling of the Rebound Step in C-H Hydroxylation by Cytochrome P450”
Eur. J. Inorg. Chem., 207-226 (2004)
<https://doi.org/10.1002/ejic.200300448>
- (244) REVIEW
 S. Shaik, P.C. Hiberty
 “Valence Bond Theory, Its History, Fundamentals, and Applications- A Primer”
Rev. Comput. Chem., **20**, 1-100 (2004)
<http://dx.doi.org/10.1002/0471678856.ch1>
- (245) L. Song, W. Wu, Q. Zhang, S. Shaik
 “A Practical Valence Bond Method: A Configuration Interaction Method Approach with Perturbation Theoretic Facility”
J. Comput. Chem., **25**, 472-478 (2004)
<https://doi.org/10.1002/jcc.10382>
- (246) D. Kumar, S.P. de Visser, P.K. Sharma, S. Cohen, S. Shaik
 “Radical Clock Substrates, Their C-H Hydroxylation Mechanism by Cytochrome P450, and Other Reactivity Patterns: What Does Theory Reveal About Clocks’ Behavior?”
J. Am. Chem. Soc., **126**, 1907-1920 (2004)
<https://doi.org/10.1021/ja039439s>
- (247) S. Kozuch, S. Shaik, A. Jutand, C. Amatore
 “Active Anionic Zero-Valent Palladium Catalysts: Characterization by Density Functional Calculations”
Chem. Eur. J., **10**, 3072-3080 (2004)
<https://doi.org/10.1002/chem.200306056>
- (248) P.K. Sharma, R. Kevorkyants, S.P. de Visser, D. Kumar, S. Shaik
 “Porphyrin Traps its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450”
Angew. Chem., Int. Ed., **43**, 1129-1132 (2004)
<https://doi.org/10.1002/anie.200352943>
Angew. Chem. **116**, 1149-1152 (2004).
- (249) H. Lin, J.C. Schöneboom, S. Cohen, S. Shaik, W. Thiel

- “QM/MM Study of the Product-Enzyme Complex in P450_{cam} Catalysis”
J. Phys. Chem. B, **108**, 10083-10088 (2004)
<https://doi.org/10.1021/jp049363z>
- (250) REVIEW
 W. Wu, L. Song, Q. Zhang, S. Shaik
 “VBCI: A Valence Bond Configuration Interaction Method that Includes Dynamic Correlation”
Encyclopedia of Computational Chemistry, Vol. 5
 P.v.R. Schleyer, N.L. Allinger, T. Clark, J. Gasteiger, H.F. Schaefer, P.R. Schreiner, Eds. Wiley-VCH,
 Chichester, 2004
<https://doi.org/10.1002/0470845015.cu0017>
 online edition. <http://www.mrw.interscience.wiley.com/ecc/articles/cu0017/abstractfs.html>
- (251) REVIEW
 B. Meunier, S.P. de Visser, S. Shaik
 “Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes”
Chem. Rev., **104**, 3947-3980 (2004)
<https://doi.org/10.1021/cr020443g>
- (252) D. Kumar, S.P. de Visser, S. Shaik
 “Oxygen Economy of Cytochrome P450: What is the Origin of the Mixed Functionality as a Dehydrogenase-Oxidase Enzyme Compared with its Normal Function?”
J. Am. Chem. Soc., **126**, 5072-5073 (2004)
<https://doi.org/10.1021/ja0318737>
- (253) L. Song, W. Wu, Q. Zhang, S. Shaik
 “VBPCM: A Valence Bond Method that Incorporates a Polarizable Continuum Model”
J. Phys. Chem. A, **108**, 6017-6024 (2004)
<https://doi.org/10.1021/jp049467c>
- (254) S. Shaik, S.P. de Visser, D. Kumar
 “External Electric Field Will Control the Selectivity of Enzymatic-Like Bond Activations”
J. Am. Chem. Soc., **126**, 11746-11749 (2004)
<https://doi.org/10.1021/ja047432k>
- (255) S. Shaik, S.P. de Visser, D. Kumar
 “One Oxidant, Many Pathways: A Theoretical Perspective of Monooxygenation Mechanisms by Cytochrome P450 Enzymes”
J. Biol. Inorg. Chem., **9**, 661-668 (2004)
<https://doi.org/10.1007/s00775-004-0576-6>
- (256) P. Su, L. Song, W. Wu, P.C. Hiberty, S. Shaik
 “Valence Bond Calculations of Hydrogen Transfer Reactions: A General Predictive Pattern Derived from Theory”
J. Am. Chem. Soc., **126**, 13539-13549 (2004)
<https://doi.org/10.1021/ja048105f>
- (257) S.P. de Visser, D. Kumar, S. Cohen, R. Shacham, S. Shaik
 “A Predictive Pattern of Computed Barriers for C-H hydroxylation by Compound I of Cytochrome P450”
J. Am. Chem. Soc., **126**, 8362-8363 (2004)
<https://doi.org/10.1021/ja048528h>
- (258) C. Amatore, A. Jutand, F. Lemarié, J.-L. Ricard, S. Kozuch, S. Shaik
 “Formation of Anionic Palladium(0) Complexes Ligated by the Trifluoroacetate Ion and their Reactivity in Oxidative Addition”
J. Organomet. Chem., **689**, 3728-3734 (2004)
<https://doi.org/10.1016/j.jorganchem.2004.05.012>

2005

- (259) S. Shaik, D. Danovich, B. Silvi, D.L. Lauvergant, P.C. Hiberty
 “Charge-Shift Bonding- A Class of Electron-Pair Bonds that Emerges from Valence Bond Theory and Is Supported by the Electron Localization Function Approach”
Chem Eur. J., **11**, 6358-6371 (2005)
<https://doi.org/10.1002/chem.200500265>
- (260) W. Wu, S. Shaik, W.H. Saunders
 “Valence Bond Calculations on the Transition state for the E2 Reaction of Fluoride ion with Ethyl Fluoride- Implications for the More O’Ferrall-Jencks Diagram”

- Can. J. Chem.*, **83**, 1649-1653 (2005)
<https://doi.org/10.1139/v05-161>
- (261) **REVIEW**
 S. Shaik, S.P. de Visser
 “Computational Approaches to Cytochrome P450 Functions”,
 in: Ortiz de Montellano, P. R., Ed. “Cytochrome P450: Structure, Mechanism and Biochemistry”,
 third ed.; Kluwer Academic Publications/Plenum Press: New York, 2005
https://doi.org/10.1007/0-387-27447-2_2
- (262) S. Kozuch, T. Leifels, D. Meyer, L. Sbaragli, S. Shaik, W.-D. Woggon
 “New Synthetic Models of Cytochrome P450: How Different are they from the Natural Species?”
SynLett., **4**, 675-684 (2005)
<https://doi.org/10.1055/s-2005-863724>
- (263) S. Shaik
 “Autobiography of Sason S. Shaik”
J. Phys. Chem. A. **112**, 12724-12736 (2008)
<https://doi.org/10.1021/jp806625w>
- (264) D. Kumar, S.P. de Visser, P.K. Sharma, E. Derat, S. Shaik
 “The Intrinsic Axial Ligand Effect on Propene Oxidation by Horseradish Peroxidase vs Cytochrome P450
 Enzymes”
J. Biol. Inorg. Chem., **10**, 181-189 (2005)
<https://doi.org/10.1007/s00775-004-0622-4>
- (265) **REVIEW**
 S. Shaik, P.C. Hiberty
 “The Valence Bond Diagram Approach: A Paradigm for Chemical Reactivity”, Chapter 23, pp 635-
 668. In: “Theory and Applications of Computational Chemistry: The First 40 Years”
 C.E. Dykstra, G. Frenking, K.S. Kim, G.E. Scuseria, Eds. Elsevier, Amsterdam, 2005
<https://doi.org/10.1016/B978-044451719-7/50066-4>
- (266) D. Kumar, S.P. de Visser, S. Shaik
 “Theory Favors a Stepwise Mechanism of Porphyrin Degradation by a Ferric Hydroxperoxide Model of the
 Active Species of Heme Oxygenase”
J. Am. Chem. Soc., **127**, 8204-8213 (2005)
<https://doi.org/10.1021/ja0446956>
- (267) D. Kumar, S.P. de Visser, P.K. Sharma, H. Hirao, S. Shaik
 “Sulfoxidation Mechanisms Catalyzed by Cytochrome P450 and Horseradish Peroxidase Models: Spin Selection
 Induced by the Ligand”
Biochemistry, **44**, 8148-8158 (2005)
<https://doi.org/10.1021/bi050348c>
- (268) **REVIEW**
 S. Shaik, D. Kumar, S.P. de Visser, A. Altun, W. Thiel,
 “Theoretical Perspective on the Structure and Mechanisms of Cytochrome P450 Enzymes”
Chem. Rev., **105**, 2279-2328 (2005)
<https://doi.org/10.1021/cr030722j>
- (269) P.C. Hiberty, S. Shaik
 “Some Answers to Frequently Asked Questions about the Distortive Tendencies of π -Electronic Systems”
Theor. Chem. Acc., **114**, 169-181 (2005)
<https://doi.org/10.1007/s00214-005-0658-8>
- (270) D. Kumar, H. Hirao, L. Que, Jr., S. Shaik
 “Theoretical Investigation of C-H Hydroxylation by (N4Py)Fe^{IV}=O²⁺: An Oxidant More Powerful than P450?”
J. Am. Chem. Soc., **127**, 8026-8027 (2005)
<https://doi.org/10.1021/ja0512428>
- (271) S. Kozuch, A. Jutand, C. Amatore, S. Shaik
 “What Makes for a Good Catalytic Cycle? A Theoretical Study of the Role of Anionic Palladium(0) Complex in
 the Cross-Coupling of an Aryl Halide with a Nucleophile”
Organometallics, **24**, 2319-2330 (2005)
<https://doi.org/10.1021/om050160p>
- (272) D. Kumar, H. Hirao, S.P. de Visser, J. Zheng, D. Wang, W. Thiel, S. Shaik
 “New Features in the Catalytic Cycle of Cytochrome P450 during the Formation of Compound I from Compound
 0”

- J. Phys. Chem. B*, **109**, 19946-19951 (2005)
<https://doi.org/10.1021/jp054754h>
- (273) E. Derat, S. Cohen, S. Shaik, A. Altun, W. Thiel
 “The Principal Active Species of Horseradish Peroxidase, Compound I: A Hybrid Quantum Mechanical/Molecular Mechanical Study”
J. Am. Chem. Soc., **127**, 13611-13621 (2005)
<https://doi.org/10.1021/ja0534046>
- (274) D. Kumar, E. Derat, A.M. Khenkin, R. Neumann, S. Shaik
 “The High-Valent Iron-Oxo Species of Polyoxometalate, if it Can Be Made, Will Be a Highly Potent Catalyst for C-H Hydroxylation and Double-Bond Epoxidation”
J. Am. Chem. Soc., **127**, 17712-17718 (2005)
<https://doi.org/10.1021/ja0542340>
- (275) H. Hirao, D. Kumar, W. Thiel, S. Shaik
 “Two-States and Two More in the Mechanisms of Hydroxylation and Epoxidation by P450”
J. Am. Chem. Soc., **127**, 13007-13018 (2005)
<https://doi.org/10.1021/ja053847+>

2006

- (276) P.C. Hiberty, C. Megret, L. Song, W. Wu, S. Shaik
 “Barriers for Hydrogen vs. Halogen Exchange: An Experimental Manifestation of Charge-Shift Bonding”
J. Am. Chem. Soc., **128**, 2836-2843 (2006) <https://doi.org/10.1021/ja053130m>
- (277) L. Song, W. Wu, P.C. Hiberty, S. Shaik
 “The Identity S_N2 Reactions $X + CH_3-X \rightarrow X-CH_3 + X$ ($X=F, Cl, Br$ and I) in Vacuum and in Aqueous Solution: A Valence Bond Study”
Chem. Eur. J., **12**, 7458-7466 (2006)
<https://doi.org/10.1002/chem.200600372>
- (278) A. Altun, S. Shaik, W. Thiel
 “Systematic QM/MM Investigation of Factors that Affect the Cytochrome P450cam - Catalyzed Hydrogen Abstraction of Camphor”
J. Comput. Chem., **27**, 1324-1337 (2006)
<https://doi.org/10.1002/jcc.20398>
- (279) S.P. de Visser, D. Kumar, M. Danovich, N. Nevo, D. Danovich, P.K. Sharma, W. Wu, S. Shaik
 “Ferromagnetic Bonding: High Spin Copper Clusters ($^{n+1}Cu_n$; $n = 2-12$) Devoid of Electron Pairs But Possessing Strong Bonding”
J. Phys. Chem. A, **110**, 8510-8518 (2006)
<https://doi.org/10.1021/jp055125a>
- (280) C. Li, W. Wu, D. Kumar, S. Shaik
 “Kinetic Isotope Effect is a Sensitive Probe of Spin State Reactivity in C-H Hydroxylation of N,N-Dimethylaniline by Cytochrome P450”
J. Am. Chem. Soc., **128**, 394-395 (2006)
<https://doi.org/10.1021/ja055987p>
- (281) M.E. Elkhani, S. Shaik
 “A Topological Study of the Ferromagnetic “No-Pair Bonding” in Maximum-Spin Lithium Clusters: $^{n+1}Li_n$ ($n=2-6$)”
Theor. Chem. Acc., **116**, 390-397 (2006)
<https://doi.org/10.1007/s00214-006-0081-9>
- (282) CHAPTER
 S. Shaik
 “A Tale of Two States”, pp 233-249.
 In “*Modeling Molecular Structure and Reactivity in Biological Systems*”
 K. Naidoo, J. Brady, M. Field, J. Gao, M. Hann, Eds. RSC Publishing, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, UK, 2006
- (283) H. Hirao, D. Kumar, L. Que, Jr., S. Shaik
 “Two-State Reactivity in Alkane Hydroxylation by Non-Heme Iron-Oxo Complexes”
J. Am. Chem. Soc., **128**, 8590-8606 (2006)
<https://doi.org/10.1021/ja061609o>
- (284) S. Cohen, D. Kumar, S. Shaik

- “In Silico Design of a Mutant of Cytochrome P450 Containing Selenocysteine”
J. Am. Chem. Soc. **128**, 2649-2653 (2006)
<https://doi.org/10.1021/ja056586c>
- (285) A. Altun, R.A. Friesner, V. Guallar, S. Shaik, W. Thiel,
 “The Effect of Heme Environment on the Hydrogen Abstraction Reaction of Camphor in P450_{cam} Catalysis: A QM/MM Study”
J. Am. Chem. Soc., **128**, 3924-3925 (2006)
<https://doi.org/10.1021/ja058196w>
- (286) G. Frenking, S. Shaik
 Foreword to the Issue “90 Years to the Lewis Concept”
J. Comput. Chem., **28**, 1-3 (2006)
- (287) D. Kumar, H. Hirao, S. Shaik, P.M. Koslowski
 “Proton-Shuffle Mechanism of O-O Activation for Formation of the High-Valent Oxo-Iron Species of Bleomycin”
J. Am. Chem. Soc., **128**, 16148-16158 (2006)
<https://doi.org/10.1021/ja064611o>
- (288) E. Derat, D. Kumar, H. Hirao, S. Shaik
 “Gauging the Relative Oxidative Powers of Compound I, Ferric-Hydroperoxide and the Ferric-Hydrogen Peroxide Species of Cytochrome P450 towards C-H Hydroxylation of a Radical Clock Substrate”
J. Am. Chem. Soc., **128**, 473-484 (2006)
<https://doi.org/10.1021/ja056328f>
- (289) S. Kozuch, S. Shaik
 “A Combined Kinetic-Quantum Mechanical Model for Assessment of Catalytic Cycles: Application to the Cross Coupling and Heck Reactions”
J. Am. Chem. Soc., **128**, 3355-3356 (2006)
<https://doi.org/10.1021/ja0559146>
- (290) E. Derat, S. Shaik
 “The Poulos-Kraut Mechanism of Compound I Formation in Horseradish Peroxidase: A QM/MM Study”
J. Phys. Chem B, **110**, 10526-10533 (2006)
<https://doi.org/10.1021/jp055412e>
- (291) H. Hirao, S. Shaik, P.M. Koslowski
 “Theoretical Analysis of the Structural and Electronic Properties of Metalloporphyrin π -Cation Radicals”
J. Phys. Chem. A, **110**, 6091-6099 (2006)
<https://doi.org/10.1021/jp0558066>
- (292) E. Derat, S. Shaik
 “Two-state Reactivity, Electromerism, Tautomerism and ‘Surprise’ \square Isomers In The Formation of Compound II of the Enzyme Horseradish Peroxidase From The Principal Species, Compound I”
J. Am. Chem. Soc., **128**, 8185-8198 (2006)
<https://doi.org/10.1021/ja0600734>
- (293) M. Ahlquist, S. Kozuch, S. Shaik, D. Tanner, P.-O. Norrby
 “Correspondence: On the Performance of Continuum Solvation Models for the Solvation Energy of Small Anions”
Organometallics, **25**, 45-47 (2006)
<https://doi.org/10.1021/om0508278>
- (294) J. Li, S. Shaik, H.B. Schlegel
 “A Single Transition State Serves Two Mechanisms. The Branching Ratio for $\text{CH}_2\text{O}^+ + \text{CH}_3\text{Cl}$ on Improved Potential Energy Surface”
J. Phys. Chem. A, **110**, 2801-2806 (2006)
<https://doi.org/10.1021/jp0563336>
- (295) E. Derat, D. Kumar, R. Neumann, S. Shaik
 “Catalysts for Monooxygenations Made From Polyoxometalate: An Iron-Oxo Derivative of the Lindqvist Anion”
Inorg. Chem., **45**, 8655-8663 (2006)
<https://doi.org/10.1021/ic0610435>
- (296) A.M. Khenkin, D. Kumar, S. Shaik, R. Neumann
 “Characterization of Manganese(V)-Oxo Polyoxometalate Intermediates and their Properties in Oxygen-Transfer Reactions”
J. Am. Chem. Soc., **128**, 15451-15460 (2006)
<https://doi.org/10.1021/ja0638455>
- (297) E. Derat, S. Shaik

- “An Efficient Proton-Coupled Electron Transfer-Process during Oxidation of Ferulic Acid by Horseradish Peroxidase: Coming a Full Cycle”
J. Am. Chem. Soc., **128**, 13940-13949 (2006)
<https://doi.org/10.1021/ja065058d>
- (298) S. Cohen, S. Kozuch, C. Hazan, S. Shaik
 “Does Substrate Oxidation Determine the Regioselectivity of Cyclohexene and Propene Oxidation by Cytochrome P450?”
J. Am. Chem. Soc., **128**, 11028-11029 (2006)
<https://doi.org/10.1021/ja063269c>
- (299) J. Zheng, D. Wang, W. Thiel, S. Shaik
 “QM/MM Study of Mechanisms for Compound I Formation in the Catalytic Cycle of Cytochrome P450”
J. Am. Chem. Soc., **128**, 13204-13215 (2006)
<https://doi.org/10.1021/ja063439l>
- (300) H. Hirao, D. Kumar, S. Shaik
 “On the Identity and Reactivity Patterns of the ‘Second Oxidant’ of T252A Mutant of Cytochrome P450_{cam} in the Oxidation of 5-Methylenylcamphor”
J. Inorg. Biochem., **100**, 2054-2068 (2006)
<https://doi.org/10.1016/j.jinorgbio.2006.09.001>
- 2007**
- (301) S. Shaik
 “Is My Chemical Universe Localized or Delocalized? Is there a Future for Chemical Concepts?”
New J. Chem., **31**, 2015-2028 (2007)
<https://doi.org/10.1039/B711641C>
- (302) P. Su, L. Song, W. Wu, P.C. Hiberty, S. Shaik
 “A Valence Bond Study of the Dioxygen Molecule”
J. Comput. Chem., **28**, 185-197 (2007)
<https://doi.org/10.1002/jcc.20490>
- (303) S. Shaik
 “The Lewis Legacy: The Chemical Bond- A Territory and Heartland of Chemistry”
J. Comput. Chem., **28**, 51-61 (2007)
<https://doi.org/10.1002/jcc.20517>
- (304) C. Hazan, D. Kumar, S.P. de Visser, S. Shaik
 “A Density Functional Study of the Factors that Influence the Regioselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes”
Eur. J. Inorg. Chem., 2966-2974 (2007)
<https://doi.org/10.1002/ejic.200700117>
- (305) P.C. Hiberty, S. Shaik
 “A Survey of Developments in *Ab Initio* Valence Bond Theory”
J. Comput. Chem., **28**, 137-151 (2007)
<https://doi.org/10.1002/jcc.20478>
- (306) P. Su, F. Ying, W. Wu, P.C. Hiberty, S. Shaik
 “The Menshutkin Reaction in the Gas Phase and in Aqueous Solution: A Valence Bond Study”
ChemPhysChem, **8**, 2603-2614 (2007)
<https://doi.org/10.1002/cphc.200700626>
- (307) K. Kühnel, E. Derat, J. Turner, S. Shaik, I. Schlichting
 “Structure and Quantum Chemical Characterization of Chloroperoxidase Compound 0, a Common Intermediate of Diverse Heme Enzymes”
Proc. Natl. Acad. Sci. U.S.A., **104**, 99-104 (2007)
<https://doi.org/10.1073/pnas.0606285103>
- (308) K.-B. Cho, Y. Moreau, D. Kumar, D.A. Rock, J.P. Jones, S. Shaik
 “Formation of the Active Species of Cytochrome P450 Using Iodosylbenzene: A Case For Spin-Selective Reactivity”
Chem. Eur. J., **13**, 4103-4115 (2007)
<https://doi.org/10.1002/chem.200601704>
- (309) S. Shaik, H. Hirao, D. Kumar
 “Reactivity Patterns of Cytochrome P450 Enzymes: Multifunctionality of the Active Species, and the Two States-Two Oxidants Conundrum”

- Nat. Prod. Rep.*, **24**, 533-552 (2007)
<https://doi.org/10.1039/B604192M>
- (310) D. Fishelovitch, C. Hazan, H. Hirao, H.J. Wolfson, R. Nussinov, S. Shaik
“QM/MM Study of the Active Species of the Human P450 3A4, and the Influence Thereof of the Multiple Substrate Binding”
J. Phys. Chem. B, **111**, 13822-13832 (2007)
<https://doi.org/10.1021/jp076401j>
- (311) Y. Wang, C. Yang, H. Wang, K. Han, S. Shaik
“A New Mechanism for Ethanol Oxidation Mediated by Cytochrome P4502E1: Bulk Polarity of the Active Site Makes the Differences”
ChemBioChem, **8**, 277-281 (2007)
<https://doi.org/10.1002/cbic.200600510>
- (312) Y. Wang, D. Kumar, C. Yang, K. Han, S. Shaik
“Theoretical Study of the N- Demethylation of Substituted *N,N*-dimethylanilines by Cytochrome P450: the Mechanistic Significance of Kinetic Isotope Effect Profiles”
J. Phys. Chem. B, **111**, 7700-7710 (2007)
<https://doi.org/10.1021/jp072347v>
- (313) Y. Moreau, H. Chen, E. Derat, H. Hirao, C. Bolm, S. Shaik
“NR Transfer Reactivity of Azo-Compound I of P450. How Does the Nitrogen Substituent Tune the Reactivity of the Species toward C-H and C=C Activation?”
J. Phys. Chem. B, **111**, 10288-10299 (2007)
<https://doi.org/10.1021/jp0743065>
- (314) P.C. Hiberty, R. Ramozzi, L. Song, W. Wu, S. Shaik
“The Physical Origin of Large Covalent-Ionic Resonance Energies in Some Two-Electron Bonds”
Faraday Discuss., **135**, 261-272 (2007)
<https://doi.org/10.1039/B605161H>
- (315) H. Hirao, D. Kumar, H. Chen, R. Neumann, S. Shaik
“The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron Transfer”
J. Phys. Chem. C, **111**, 7711-7719 (2007)
<https://doi.org/10.1021/jp068673c>
- (316) K.-B. Cho, E. Derat, S. Shaik
“Compound I of Nitric Oxide Synthase: The Active Site Protonation State”
J. Am. Chem. Soc., **129**, 3182-3188 (2007)
<https://doi.org/10.1021/ja066662r>
- (317) E. Derat, S. Shaik, C. Rovira, P. Vidossich, M. A- Prieto
“The Effect of a Water Molecule on the Mechanism of Formation of Compound 0 in Horseradish Peroxidase”
J. Am. Chem. Soc., **129**, 6346-6347 (2007)
<https://doi.org/10.1021/ja0676861>
- (318) S. Shaik, H. Hirao, D. Kumar
“Reactivity of High-Valent Iron-Oxo Species in Enzymes and Synthetic Reagents: A Tale of Many States”
Acc. Chem. Res., **40**, 532-542 (2007)
<https://doi.org/10.1021/ar600042c>
- (319) D. Fishelovitch, S. Shaik, H.J. Wolfson, R. Nussinov
“Structural Dynamics of the Cooperative binding of Organic Molecules in the Human Cytochrome P4503A4”
J. Am. Chem. Soc., **129**, 1602-1611 (2007)
<https://doi.org/10.1021/ja066007j>
- (320) A. Altun, S. Shaik, W. Thiel
“What is the Active Species of Cytochrome P450 during Camphor Hydroxylation? QM/MM studies of Different Electronic States of Compound I and of Reduced and Oxidized Iron-Oxo Intermediates”
J. Am. Chem. Soc., **129**, 8978-8987 (2007)
<https://doi.org/10.1021/ja066847y>
- (321) C. Li, L. Zhang, C. Zhang, H. Hirao, W. Wu, S. Shaik
“Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?”
Angew. Chem., Int. Ed., **46**, 8168-8170 (2007)
<https://doi.org/10.1002/anie.200702867>
- (322) C.V. Sastri, J. Lee, K. Oh, Y.J. Lee, J. Lee, T.A. Jackson, K. Ray, H. Hirao, W. Shin, J.A. Halfen, J. Kim, L. Que, Jr., S. Shaik, W. Nam
“Axial Ligand Tuning of a Nonheme Iron(IV)-Oxo Unit for Hydrogen Atom Abstraction”

- Proc. Natl. Acad. Sci. U.S.A.*, **104**, 19181-19186 (2007)
<https://doi.org/10.1073/pnas.0709471104>
- (323) M. Unno, H. Chen, S. Kusama, S. Shaik, M. Ikeda-Saito
 “Structural Characterization of the Fleeting Ferric Peroxo Species in Myoglobin: Experiment and Theory”
J. Am. Chem. Soc., **129**, 13394-13395 (2007)
<https://doi.org/10.1021/ja076108x>
- 2008**
- (324) S. Shaik, D. Kumar, S.P. de Visser
 “A Valence Bond Modeling of Trends in Hydrogen Abstraction Barriers and Transition States of Hydroxylation Reactions Catalyzed by Cytochrome P450 Enzymes”
J. Am. Chem. Soc., **130**, 10128-10140 (2008); **130**, 14016 (2008) (Correction)
<https://doi.org/10.1021/ja8019615>
- (325) P. Su, L. Song, W. Wu, S. Shaik, P.C. Hiberty
 “Heterolytic Bond Dissociation in Water: Why So Easy for C₄H₉Cl but Not for C₃H₉SiCl?”
J. Phys. Chem. A, **112**, 2988-2997 (2008)
<https://doi.org/10.1021/jp8004647>
- (326) H. Hirao, K. B. Cho, and S. Shaik
 “QM/MM Theoretical Study of the Pentacoordinate Mn(III) and Resting States of Manganese-Reconstituted Cytochrome P450_{cam}”
J. Biol. Inorg. Chem., **13**, 521-530 (2008)
<https://doi.org/10.1007/s00775-007-0340-9>
- (327) S. Kozuch, S. Shaik
 “Kinetic-Quantum Chemical Model for Catalytic Cycles: The Haber-Bosch Process and the Effect of Reagents Concentration”
J. Phys. Chem. A, **112**, 6032-6041 (2008)
<https://doi.org/10.1021/jp8004772>
- (328) H. Hirao, L. Que, Jr., W. Nam, S. Shaik
 “A Two-State Reactivity Rationale for Counterintuitive Axial Ligand Effects on the C-H Activation Reactivity of Nonheme Fe^{IV}=O Oxidants”
Chem. Eur. J., **14**, 1740-1756 (2008)
<https://doi.org/10.1002/chem.200701739>
- (329) K.-B. Cho, H. Hirao, H. Chen, M.A. Carvajal, S. Cohen, E. Derat, W. Thiel, S. Shaik
 “Compound I in Heme Thiolate Enzymes: A Comparative QM/MM Study”
J. Phys. Chem. A, **112**, 13128-13138 (2008)
<https://doi.org/10.1021/jp806770y>
- (330) H. Chen, Y. Moreau, E. Derat, S. Shaik
 “Quantum Mechanical/Molecular Mechanical Study of Mechanisms of Heme Degradation by the Enzyme Heme Oxygenase: The Strategic Function of the Water Cluster”
J. Am. Chem. Soc., **130**, 1953-1965 (2008)
<https://doi.org/10.1021/ja076679p>
- (331) C. Li, L. Zhang, C. Zhang, W. Wu, H. Hirao, S. Shaik
 Corrigendum: “Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?”
Angew. Chem. Int. **47**, 8148 (2008)
<https://doi.org/10.1002/anie.200890215>
- (332) H. Hirao, H. Chen, M.A. Carvajal, Y. Wang, S. Shaik
 “Effect of External Electric Fields on the C-H Bond Activation Reactivity of Nonheme Iron-Oxo Reagents”
J. Am. Chem. Soc., **130**, 3319-3327 (2008)
<https://doi.org/10.1021/ja070903t>
- (333) D. Wang, J. Zheng, W. Thiel, S. Shaik
 “Quantum and Molecular Mechanical Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450_{cam} and its Mutant D251N”
J. Phys. Chem. B, **112**, 5126-5138 (2008)
<https://doi.org/10.1021/jp074958t>
- (334) Y. Wang, H. Hirao, H. Chen, H. Onaka, S. Nagano, S. Shaik
 “Electron Transfer Activation of Chromopyrrolic Acid by Cytochrome P450 En Route to the Formation of the Antitumor Indolcarbazole Derivative: Theory Supports Experiment”
J. Am. Chem. Soc., **130**, 7170-7171 (2008)

- <https://doi.org/10.1021/ja711426y>
- (335) S.N. Dhuri, M.S. Seo, Y.-M. Lee, H. Hirao, Y. Wang, W. Nam, S. Shaik
 “Experiment and Theory Reveal the Fundamental Difference between Two-State and Single-State Reactivity Patterns in Nonheme Fe^{IV}=O and Ru^{IV}=O Oxidants”
Angew. Chem. Int., Ed., **47**, 3356-3359 (2008)
<https://doi.org/10.1002/anie.200705880>
- (336) H. Chen, M. Ikeda-Saito, S. Shaik
 “Nature of the Fe–O₂ Bonding in Oxy–Myoglobin: Effect of the Protein”.
J. Am. Chem. Soc., **130**, 14778-14790 (2008)
<https://doi.org/10.1021/ja805434m>
- (337) P. Su, W. Wu, S. Shaik, P.C. Hiberty
 “A Valence Bond Study of Low-Lying States of the NF Molecule”
Chem. Phys. Chem., **9**, 1442-1452 (2008)
<https://doi.org/10.1002/cphc.200800143>
- (338) H. Chen, H. Hirao, E. Derat, I. Schlichting, S. Shaik
 “Quantum Mechanical/Molecular Mechanical Study on the Mechanisms of Compound I Formation in the Catalytic Cycle of Chloroperoxidase: An Overview on Heme Enzymes”
J. Phys. Chem. B, **112**, 9490-9500 (2008)
<https://doi.org/10.1021/jp803010f>
- (339) J. Gu, Y. Lin, B. Ma, W. Wu, S. Shaik
 “Covalent Excited States of Polyenes C_{2n}H_{2n+2} (n = 2-8) and Polyenyl Radicals C_{2n-1}H_{2n+1} (n = 2-8): An Ab Initio Valence Bond Study”
J. Chem. Theo. Comput. **4**, 2101-2107 (2008)
<https://doi.org/10.1021/ct800341z>
- (340) **BOOK:**
 S. Shaik, P.C. Hiberty
 “*A Chemist’s Guide to Valence Bond Theory*”
 pp. 1-316.
 1st Edition: Wiley-Interscience, 2008
<https://doi.org/10.1002/9780470192597>
- 2009**
- (341) Z. Chen, J. Song, S. Shaik, P.C. Hiberty, W. Wu,
 “Valence Bond Perturbation Theory. A Valence Bond Method that Incorporates Perturbation Theory”
J. Phys. Chem. A, **113**, 11560-11569 (2009)
<https://doi.org/10.1021/jp903011j>
- (342) L. Zhang, F. Ying, W. Wu, P.C. Hiberty, S. Shaik
 “Topology of Electron Charge Density for Chemical Bonds from Valence Bond Theory: A Probe of Bonding Types”
Chem. Eur. J., **15**, 2979-2989 (2009)
<https://doi.org/10.1002/chem.200802134>
- (343) C. Li, W. Wu, K.B. Cho, S. Shaik
 “Oxidation of Tertiary Amines by Cytochrome P450 – Kinetic Isotope Effect as a Spin-State Reactivity Probe”
Chem. Eur. J. **15**, 8492-8503 (2009)
<https://doi.org/10.1002/chem.200802215>
- (344) S. Kozuch, S. E. Lee, S. Shaik
 “Theoretical Analysis of the Catalytic Cycle of a Nickel Cross-Coupling Process: Application of the Energetic Span Model”
Organometallics, **28**, 1303-1308 (2009)
<https://doi.org/10.1021/om800772g>
- (345) Y. Jiang, S. Sivaramakrishnan, T. Hayashi, S. Cohen, P. Moenne-Loccoz, S. Shaik, P.R. Ortiz de Montellano
 “Calculated and Experimental Spin State of Seleno Cytochrome P450”.
Angew. Chem. Int. Ed., **48**, 7193-7195 (2009)
<https://doi.org/10.1002/anie.200901485>
- (346) E.J. Klinker, H. Hirao, S. Shaik, L. Que, Jr.
 “A Two-State Reactivity Model Explains Unusual Kinetic Isotope Effect Patterns in C-H Bond Cleavage by Nonheme Oxoiron(IV) Complexes.”
Angew. Chem. Int. Ed. **48**, 1291-1295 (2009)

- <https://doi.org/10.1002/anie.200804029>
- (347) K.B. Cho, M.A. Carvajal, S. Shaik
 “First Half-Reaction Mechanism of Nitric Oxide Synthase: The Role of Proton and Oxygen Coupled Electron Transfer in the Reaction by Quantum Mechanics/Molecular Mechanics.”
J. Phys. Chem. B. **113**, 336-346 (2009)
<https://doi.org/10.1021/jp8073199>
- (348) W. Wu, J. Gu, J. Song, S. Shaik, P.C. Hiberty
 “The Inverted Bond in [1.1.1] Propellane is a Charge-Shift Bond”
Angew. Chem. Int. Ed. **48**, 1407-1410 (2009)
<https://doi.org/10.1002/anie.200804965>
- (349) D. Fishelovitch, S. Shaik, H.J. Wolfson, R. Nussinov
 “Theoretical Characterization of Substrate Access/Exit Channels in the Human Cytochrome P450 3A4 Enzyme: Involvement of Phenylalanine Residues in the Gating Mechanism”.
J. Phys. Chem. B. **113**, 13018-13025 (2009)
<https://doi.org/10.1021/jp810386z>
- (350) Y. Kang, H. Chen, Y. J. Jeong, W. Lai, E. H. Bae, S. Shaik and W. Nam
 “Enhanced Reactivities of Iron(IV)-Oxo Porphyrin π -Cation Radicals in Oxygenation Reactions by Electron-Donating Axial Ligands ”
Chem. Eur. J. **15**, 10039-10046 (2009)
<https://doi.org/10.1002/chem.200901238>
- (351) I. Iraklii Ebralidze, G. Leitus, L.J.W. Shimon, Y. Wang, S. Shaik, R. Neumann
 “Structural variability in Manganese(II) Complexes of N,N'-Bis(2-pyridinylmethylene) Ethane (and Propane) Diamine Ligands”
Inorg. Chim. Acta. **362**, 4713-4720 (2009)
<https://doi.org/10.1016/j.ica.2009.06.037>
- (352) S. Shaik, D. Danovich, W. Wu, P.C. Hiberty,
 “Charge-shift Bonding and its Manifestations in Chemistry”
Nature Chem. **1**, 443-449 (2009)
<https://doi.org/10.1038/nchem.327>
- (353) W. Lai, H. Chen, K.-B. Cho, S. Shaik,
 “Effects of Substrate, Protein Environment and Proximal Ligand Mutation of Compound I and Compound 0 of Chloroperoxidase”
J. Phys. Chem. A. **113**, 11763-17771 (2009)
<https://doi.org/10.1021/jp902898s>
- (354) S. Shaik, Z. Chen, W. Wu, A. Stanger, D. Danovich, P.C. Hiberty
 “An Excursion from Normal to Inverted C-C Bonds Shows a Clear Demarcation between Covalent and Charge-Shift C-C Bonds”
ChemPhysChem, **10**, 2658-2669 (2009)
<https://doi.org/10.1002/cphc.200900633>
- (355) M.A. Carvajal, S. Kozuch, S. Shaik
 “Factors Controlling the Selective Hydroformylation of Internal Alkenes to Linear Aldehydes. 1. The Isomerization Step”.
Organometallics, **28**, 3656-3665 (2009)
<https://doi.org/10.1021/om801166x>
- (356) W. Lai, H. Chen, S. Shaik
 “What Kinds of Ferryl Species Exist for Compound II of Chloroperoxidase? A Dialog of Theory with experiment”
J. Phys. Chem. B. **113**, 7912-7917 (2009)
<https://doi.org/10.1021/jp902288q>

2010

- (357) W. Lai, H. Chen, K.-B. Cho, S. Shaik
 “External Electric Field Can Control the Catalytic Cycle of Cytochrome P450_{cam}: A QM/MM Study”
J. Phys. Chem. Lett. **1**, 2082-2087 (2010)
<https://doi.org/10.1021/jz100695n>
- (358) D. Danovich, S. Shaik
 “Bound Triplet Pairs in the Highest Spin States of Coinage Metal Clusters”

- J. Chem. Theory Comput.* **6**, 1479-1489 (2010)
<https://doi.org/10.1021/ct100088u>
- (359) W. Wu, S. Shaik, W.H. Saunders
 “VBSCF Calculations on the Bimolecular (E2) Elimination Reaction. The Nature of the Transition State”.
J. Org. Chem. **75**, 3722-3728 (2010)
<https://doi.org/10.1021/jo100465j>
- (360) S. Shaik, S. Cohen, Y. Wang, H. Chen, D. Kumar, and W. Thiel
 “P450 Enzymes: Their Structure, Reactivity and Selectivity- Modeled by QM/MM Calculations”
Chem. Rev. **110**, 949-1017 (2010)
<https://doi.org/10.1021/cr900121s>
- (361) D. Fishelovitch, S. Shaik, H.J. Wolfson, R. Nussinov
 “How Does the Reductase Help to Regulate the Catalytic Cycle of Cytochrome P450 3A4 Using the Conserved Water Channel?”
J. Phys. Chem B, **114**, 5964-5970 (2010)
<https://doi.org/10.1021/jp101894k>
- (362) Y. Wang, L. Dongmei, K. Han, S. Shaik
 “An Acyl Group Makes a Difference in the Reactivity Patterns of Cytochrome P450 Catalyzed N-Demethylation of Substituted N,N-Dimethyl Benzamides - High Spin Selective Reactivity”.
J. Phys. Chem. B, **114**, 2964-2970 (2010)
<https://doi.org/10.1021/jp9097974>
- (363) P. Vidossich, G. Fiorini, M. Alfonso-Prieto, E. Derat, S. Shaik, C. Rovira
 “On the Role of Water in Peroxidase Catalysis: A Theoretical Investigation of HRP Compound I Formation”
J. Phys. Chem. B, **114**, 5161-5169 (2010)
<https://doi.org/10.1021/jp911170b>
- (364) S. Shaik, Y. Wang, H. Chen, J. Song, R. Meir
 “Valence Bond Modeling and Density Functional Theory Calculations of Reactivity and Mechanism of Cytochrome P450 Enzymes: Thioether Sulfoxidation”.
Faraday Discuss., **145**, 49-70 (2010)
<https://doi.org/10.1039/B906094D>
- (365) R. Meir, H. Chen, W. Lai, S. Shaik
 “Oriented Electric Fields Accelerate the Diels-Alder Reactions and Control the Endo/Exo Selectivity”.
ChemPhysChem, **11**, 301-310 (2010)
<https://doi.org/10.1002/cphc.200900848>
- (366) H. Chen, J. Song, W.Z. Lai, W. Wu and S. Shaik
 “Multiple Low-Lying States for Compound I of P450_{cam} and Chloroperoxidase Revealed from Multireference Ab Initio QM/MM Calculations”. [Selected for issue cover]
J. Chem. Theory Comput. **6**, 940-953 (2010).
<https://doi.org/10.1021/ct9006234>
- (367) S. Kozuch, S. Shaik
 “Defining the Optimal Inductive and Steric Requirements for a Cross-Coupling Catalyst Using the Energetic Span Model”.
J. Mol. Catal. A: **324**, 120-126 (2010)
<https://doi.org/10.1016/j.molcata.2010.02.022>
- (368) D. Janardanan, Y. Wang, P. Schyman, L. Que Jr., S. Shaik
 “The Fundamental Role of Exchange-Enhanced Reactivity in C-H Activation by S=2 Oxo iron(IV) Complexes”.
Angew. Chem. Int. Ed. **49**, 3342-3345 (2010)
<https://doi.org/10.1002/anie.201000004>
- (369) P. Schyman, D. Usharani, Y. Wang, S. Shaik
 “Brain Chemistry: How Does P450 Catalyze the O-Demethylation Reaction of 5-Methoxytryptamine to Yield Serotonin?” [Selected for issue cover]
J. Phys. Chem B, **114**, 7078-7089 (2010).
<https://doi.org/10.1021/jp1008994>
- (370) S. Shaik
 Report on: “Encyclopedia of Inorganic Chemistry: Computational Inorganic and Bioinorganic Chemistry”, E.I. Solomon, R.A. Scott, R.B. King, Eds., Wiley and Sons, Hoboken 2009.
Angew. Chem. Int. Ed. **49**, 3111-3113 (2010);
 German Edition: *Angew. Chem.* **122**, 3177-3179 (2010)
- (371) S. Shaik
 “Valence Bond All the Way: From the Degenerate H-Exchange to Cytochrome P450”

- Phys. Chem. Chem. Phys.* **12**, 8706-8720 (2010)
<https://doi.org/10.1039/C001372M>
- (372) S.C. Sawant, X. Wu, J. Cho, K.-B. Cho, S.H. Kim, M.S. Seo, Y.M. Lee, M. Kubo, T. Ogura, S. Shaik, W. Nam. "Water as an Oxygen source: Synthesis, Characterization, and Reactivity Studies of a Mononuclear Nonheme Manganese(IV) Oxo Complex"
Angew. Chem. Int. Ed. **49**, 8190-8194 (2010)
<https://doi.org/10.1002/anie.201000819>
- (373) W. Z. Lai, H. Chen, T. Matsui, K. Omori, M. Unno, M. Ikeda-Saito, S. Shaik
 "Enzymatic Ring Opening Mechanism of Verdoheme by the Heme Oxygenase: A Combined X-ray Crystallography and QM/MM Study"
J. Am. Chem. Soc. **132**, 12960-12970 (2010)
<https://doi.org/10.1021/ja104674q>
- (374) S. Shaik, W.Z. Lai, H. Chen, Y. Wang
 "The Valence Bond Way: Reactivity Patterns of Cytochrome P450 Enzymes and Synthetic Analogs"
Acc. Chem. Res. **43**, 1154-1165 (2010)
<https://doi.org/10.1021/ar100038u>
- (375) S. Shaik, and Yuandi Li, Interview: "The Magic of Chemistry",
Highlights in Chemical Technology, November 30th Issue 12, 2010
http://www.rsc.org/Publishing/ChemTech/Volume/2010/12/sason_shaik_interview.asp
 See also, the Faraday Discussion Blog:
<http://blogs.rsc.org/fd/2010/12/02/interview-with-sason-shaik-the-magic-of-chemistry/>
 in the HTML form (http://www.rsc.org/Publishing/ChemTech/Volume/2010/12/sason_shaik_interview.asp) and
 as an "online magazine" (<http://mag.digitalpc.co.uk/olive/ode/hchemtech/>).

2011

- (376) E. Ploshnik, D. Danovich, P.C. Hiberty, S. Shaik
 "The Nature of the Idealized Triple Bonds Between Principal Elements, and the σ Origins of Trans-Bent Geometries- A Valence Bond Study".
J. Chem. Theor. Comput. **7**, 955-968 (2011)
<https://doi.org/10.1021/ct100741b>
- (377) D. Kumar, A. Altun, S. Shaik, W. Thiel
 "Water as a Biocatalyst in Cytochrome P450"
Faraday Discussions, **148**, 373-383 (2011)
<https://doi.org/10.1039/C004950F>
- (378) K.B. Cho, W.Z. Lai, M. Hamberg, C.S. Raman, S. Shaik
 "The Reaction Mechanism of Allene Oxide Synthase: Interplay of Theoretical QM/MM Calculations and Experimental Investigations".
Arch. Biochem. Biophys. **507**, 14-25 (2011)
<https://doi.org/10.1016/j.abb.2010.07.016>
- (379) P. Su, J. Wu, J. Gu, W. Wu, S. Shaik, P.C. Hiberty
 "Bonding Conundrums in the C₂ Molecule: A Valence Bond Study"
J. Chem. Theor. & Comput. **7**, 121-130 (2011)
<https://doi.org/10.1021/ct100577v>
- (380) W. Wu, P. Su, S. Shaik, P.C. Hiberty
 "Classical Valence Bond Approach by Modern Methods".
Chem. Rev. **111**, 7557-7593 (2011)
<https://doi.org/10.1021/cr100228r>
- (381) R. Meir, S. Kozuch, A. Uhe, S. Shaik
 "How Can Theory Predict the Selectivity of Palladium-Catalyzed Cross-Coupling of Pristine Aromatic Molecules?"
Chemistry- Eur. J. **17**, 7623-7631 (2011).
<https://doi.org/10.1002/chem.200>
- (382) J. Echeverria, G. Aullon, D. Danovich, S. Shaik, S. Alvarez
 "Dihydrogen Contacts in Alkanes are Subtle But not Faint".
Nature Chem. **3**, 323- 330 (2011)
<https://doi.org/10.1038/nchem.1004>
- (383) A. Uhe, S. Kozuch, S. Shaik

- “Automatic Analysis of Computed Catalytic Cycles”
J. Comput. Chem. **32**, 978-985 (2011)
<https://doi.org/10.1002/jcc.21669>
- (384) S. Kozuch, S. Shaik
 “How to Conceptualize Catalytic Cycles? The Energetic Span Model”
Acc. Chem. Res. **44**, 101-110 (2011)
<https://doi.org/10.1021/ar1000956>
- (385) S. Shaik, P.C. Hiberty
 “A Primer on Qualitative Valence Bond Theory- A Theory Coming of Age”
WIREs Comput. Mol. Sci., **1**, 18-29 (2011)
<https://doi.org/10.1002/wcms.7>
- (386) P. Schyman, W.Z. Lai, H. Chen, Y. Wang, S. Shaik
 “The Directive of the Protein: How does Cytochrome P450 Select the Mechanism of Dopamine Formation?”
J. Am. Chem. Soc. **133**, 7977-7984 (2011)
<https://doi.org/10.1021/ja201665x>
- (387) S. Shaik, H. Chen, D. Janardanan
 “Exchange-Enhanced Reactivity in Bond Activation by Metal-Oxo Enzymes and Synthetic Reagents”
Nature Chem. **3**, 19-27 (2011).
<https://doi.org/10.1038/nchem.943>
Nature Chem. **4**, 511 (2012). Corrigendum
- (388) S. Shaik, P. Milko, P. Schyman, U. Dandamundi, H. Chen,
 “Trends in Aromatic Oxidation Catalyzed by Cytochrome P450 Enzymes: A Valence Bond Modeling”
J. Chem. Theory Comput. **7**, 327-339 (2011)
<https://doi.org/10.1021/ct100554g>
- (389) M.S. Seo, N.H. Kim, K.-B. Cho, J.E. So, S.K. Park, M. Clemancy, R. Garcia-Serras, J.-M. Latour, S. Shaik, W. Nam
 “A Mononuclear Nonheme Iron(IV)-Oxo Complex Which Is More Reactive than Cytochrome P450 Model Compound I”
Chemical Science. **2**, 1039-1045 (2011)
<https://doi.org/10.1039/C1SC00062D>
- (390) CHAPTER
 P.C. Hiberty, S. Shaik
 “Modern Ab initio Valence Bond Methods”
 Chapter 8 in: P.A. A. Popellier, Ed., “*Solving the Schrödinger equation: has everything been tried?*”
 ImperialCollege Press., World Scientific Publishing Co., London, 2011, pp. 202-236
https://doi.org/10.1142/9781848167254_0008
- (391) D. Usharani, D. Janardanan, S. Shaik
 “Does the TauD Enzyme always Hydroxylate Alkanes, while an Analogous Synthetic Non-heme Reagent always Desaturates them?”
J. Am. Chem. Soc. **133**, 176-179 (2011)
<https://doi.org/10.1021/ja107339h>
- (392) S. Shaik, H. Chen
 “Lessons on O₂ and NO Bonding to Heme from Ab Initio Multireference/Multiconfiguration and DFTcalculations”
J. Biol. Inorg. Chem. **16**, 841-855 (2011)
<https://doi.org/10.1007/s00775-011-0763-1>
- (393) W.Z. Lai, H. Chen, S. Cohen, S. Shaik,
 “Will P450_{cam} Hydroxylate or Desaturate Alkanes? QM and QM/MM Studies”.
J. Phys. Chem. Lett. **2**, 2229-2235 (2011)
<https://doi.org/10.1021/jz2007534>
- (394) H. Chen, W.Z. Lai, S. Shaik
 “Multireference and Multiconfiguration Ab Initio methods in Heme-Related Systems: What Have We Learned So Far?”
J. Phys. Chem. B. **115**, 1727-1742 (2011).
<https://doi.org/10.1021/jp110016u>
- (395) W.Z. Lai, S. Shaik
 “Can Ferric-Superoxide Act as a Potential Oxidant in P450_{cam}? QM/MM Investigation of Hydroxylation, Epoxidation, and Sulfoxidation”
J. Am. Chem. Soc. **133**, 5444-5452 (2011)

- (396) <https://doi.org/10.1021/ja111376n>
D. Schröder, S. Shaik
“Comment on ‘A Low-Spin Ruthenium(IV)-Oxo Complex: Does the Spin State Have an Impact on the Reactivity?’”
Angew. Chem. Int. Ed. **50**, 3850-3851 (2011)
<https://doi.org/10.1002/anie.201007636>
- (397) H. Chen, W.Z. Lai, J. Yao, S. Shaik
“Perferryl Fe^V-Oxo Non-heme Complexes: Do They Have High-Spin or Low-Spin Ground States?”
J. Chem. Theory Comput. **7**, 3049-3053 (2011)
<https://doi.org/10.1021/ct200614g>
- (398) N. Lühmann, H. Hirao, S. Shaik, T. Müller
“Disilylfluoronium Ions- Synthesis, Structure and Bonding”
Organometallics, **30**, 4087-4096 (2011)
<https://doi.org/10.1021/om2003128>
- (399) D. Janardanan, D. Usharani, H. Chen, S. Shaik
“Modeling C-H Abstraction Reactivity of nonheme Fe(IV)O Oxidants with Alkanes: What Role do Counter Ions Play?”
J. Phys. Chem. Lett. **2**, 2610-2617 (2011)
<https://doi.org/10.1021/jz201224x>
- (400) S. Shaik, Interview in the Blog “The Sceptical Chymist” in Nature Chemistry
May 13, 2011, Nature Chemistry, [Read Now](http://blogs.nature.com/thesepticalchymist/2011/05/reactions_sason_shaik.html)
http://blogs.nature.com/thesepticalchymist/2011/05/reactions_sason_shaik.html
- (401) R. Kang, H. Chen, S. Shaik, J. Yao
“Assessment of Theoretical Methods for Complexes of Gold(I) and Gold(III) with Unsaturated Aliphatic Hydrocarbon: Which Density Functional Should we Choose?”
J. Chem. Theory Comput. **7**, 4002-4012 (2011)
<https://doi.org/10.1021/ct200656p>

2012

- (402) S. Shaik
Highlight on “Steric Crowding Can Stabilize a Labile Molecule: Solving the Hexaphenylethane Riddle” (S. Grimme, P.R. Schreiner, *Angew. Chem. Int. Ed.* **50**, 12639, 2011).
Computational Chemistry Highlights, April 17th, 2012.
- (403) R. Mas-Balleste, A.R. McDonalld, D. Reed, D. Usharani, P. Schyman, P. Milko, S. Shaik, L. Que, Jr.
“Intramolecular Gas-Phase Reactions of Synthetic Nonheme Oxoiron(IV) Ions: Proximity and Spin-State Reactivity Rules”
Chem.–Eur. J. **18**, 11747-11760 (2012)
<https://doi.org/10.1002/chem.201200105>
- (404) S. Shaik
Nachr. Chem. **60**, 1185-1186 (2012).
Interview on the occasion of the August-Wilhelm von Hoffmann Award (Interviewer: Christian Remenyi for Nachrichten aus der Chemie).
- (405) D. Usharani, C. Zazza, L. W.Z. Lai, M. Chursaria, L. Waskell, S. Shaik
“A Single-Site Mutation (F429H) Converts the Enzyme CYP 2B4 to a Heme-Oxygenase: A QM/MM Study”.
J. Am. Chem. Soc., **134**, 4053-4056 (2012)
<https://doi.org/10.1021/ja211905e>
- (406) S. Shaik, D. Danovich, W. Wu, P. Su, H.S. Rzepa, P.C. Hiberty
“Quadruple Bonding in C₂ and Analogous Eight-Valence Electron Species”
Nature Chem. **4**, 195-200 (2012)
<https://doi.org/10.1038/nchem.1263>
- (407) K.B. Cho, E.J. Kim, M.S. Seo, S. Shaik, W. Nam
“Correlating DFT- Calculated Energy Barriers to Experiments in Nonheme Octahedral Fe^{IV}O species”
Chem. Eur. J. **18**, 10444-10453 (2012)
<https://doi.org/10.1002/chem.201200096>
- (408) W.Z. Lai, C. Li, H. Chen, S. Shaik
“Hydrogen-Abstraction Reactivity Patterns from A to Y: The Valence Bond Way”
Angew. Chem. Int. Ed. **51**, 5556-5578 (2012).

- <https://doi.org/10.1002/anie.201108398>
- (409) P.C. Hiberty, F. Volatron, S. Shaik
“In Defence of the Hybrid Atomic Orbitals”
J. Chem. Ed. **89**, 575-577 (2012)
<https://doi.org/10.1021/ed200615j>
- (410) F. Ying, P. Su, Z. Chen, S. Shaik, W. Wu
“DFVB: A Density-Functional-Based Valence Bond Method”
J. Chem. Theory Comput. **8**, 1608-1615 (2012)
<https://doi.org/10.1021/ct200803h>
- (411) D. Janardanan, U. Dandamudi, S. Shaik
“The Origins of Dramatic Axial Ligand Effects: Closed-Shell Mn^{VO} Complexes use Exchange-Enhanced Open Shell Sates to Mediate Efficient H-Abstraction Reactions”
Angew. Chem. Int. Ed. **51**, 4421-4425 (2012)
<https://doi.org/10.1002/anie.201200689>
- (412) C. Li, D. Danovich, S. Shaik
“Blended Hydrogen Atom Abstraction and Proton-Coupled Electron Transfer Mechanisms of Closed-Shell Molecules”
Chem. Sci. **3**, 1903-1918 (2012)
<https://doi.org/10.1039/C2SC20115A>
- (413) K.B. Cho, H. Chen, D. Janardanan, S.P. de Visser, S. Shaik, W. Nam
“Nonheme Iron-Oxo and -Superoxo Reactivities: O₂ Binding and Spin Inversion Probability Matter”
Chem. Commun. **48**, 2189-2191 (2012)
<https://doi.org/10.1039/C2CC17610F>
- (414) H. Chen, K.-B. Cho, W.Z. Lai, W. Nam, S. Shaik
“Dioxygen Activation by a Non-Heme Iron(II) Complex: Theoretical Study toward Understanding Ferric-Superoxo Complexes”
J. Chem. Theory Comput. **8**, 915-926 (2012)
<https://doi.org/10.1021/ct300015y>
- (415) K. Chen, G. Zhang, H. Chen, J. Yao, D. Danovich, S. Shaik
“Spin-Orbit Coupling and Outer-Core Correlation Effects in Ir- and Pt-Catalyzed C-H Activation”
J. Chem. Theory Comput. **8**, 1641-1645 (2012)
<https://doi.org/10.1021/ct3000537>
- (416) K.-B. Cho, S. Shaik, W. Nam
“Theoretical Investigation into C-H Bond Activation Reactions by Nonheme Mn^{IVO} Complexes. MultiState Reactivity with No Oxygen Rebound”
J. Phys. Chem. Lett. **3**, 2851-2856 (2012)
<https://doi.org/10.1021/jz301241z>
- (417) R. Kang, W.Z. Lai, J. Yao, S. Shaik, H. Chen
“How Accurate Can a Local Coupled Cluster Approach Be in Computing the Activation Energies of Late-Transition-Metal-Catalyzed Reactions with Au, Pt, and Ir?”
J. Chem. Theory Comput. **8**, 3119-3127 (2012).
<https://doi.org/10.1021/ct3003942i>
- (418) W.Z. Lai, R. Cao, G. Dong, S. Shaik, J. Yao, H. Chen
“Why is Cobalt the Best Transition Metal in Transition-Metal Hangman Corroles for O-O Bond Formation during Water Oxidation?”
J. Phys. Chem. Lett. **3**, 2315-2319 (2012)
<https://doi.org/10.1021/jz3008535>
- (419) W.Z. Lai, J. Yao, S. Shaik, H. Chen
“Which Density Functional Is the Best in Computing C-H Activation Energies by Pincer Complexes of Late Platinum Group Metals?”
J. Comput. Chem. **8**, 2991-2996 (2012)
<https://doi.org/10.1021/ct3005936>
- (420) K.-B. Cho, X. Wu, Y.-M. Lee, Y. H. Kwon, S. Shaik, W. Nam
“Evidence for an Alternative to the Oxygen Rebound Mechanism in C-H Bond Activation by Non-heme Fe^{IVO} Complexes”
J. Am. Chem. Soc. **134**, 20222-020225 (2012)
<https://doi.org/10.1021/ja308290r>
- (421) B. Braida, E. Derat, S. Humbel, P.C. Hiberty, S. Shaik
“The Valence Bond Workshop in Paris: The Phoenix Rises from the Ashes or, Has a Love Story eith MO-Based

- Theories Begun?
ChemPhysChem **13**, 4029-4030 (2012)
<https://doi.org/10.1002/cphc.201200784>
- (422) S. Shaik
 “The Ups and Downs of Chemistry” A Brief Interview on Occasion of the August-Wilhelm von Hofmann Medal Award
ChemPhysChem, **13**, 3082-3083 (2012).
- (423) S. Shaik, D. Danovich
 “A Comment on: A Paramagnetic Bonding Mechanism in Strong Magnetic Fields”.
Computational Chemistry Highlights, August 17th, 2012.

2013

- (424) D. Danovich, S. Shaik, F. Neese, J. Echeverria, G. Aullon, S. Alvarez
 “Understanding the Nature of the CH \cdots HC Interactions in Alkanes”.
J. Chem. Theor. Comput. **9**, 1977-1991 (2013)
<https://doi.org/10.1021/ct400070j>
- (425) CHAPTER
 D. Danovich, S. Shaik, H. Chen
 “Theoretical Toolkits for Inorganic and Bioinorganic Complexes: Their Application and Insights”
 Invited Chapter, in,
 “*Comprehensive Inorganic Chemistry II*”, Vol. 9; Chapter 1, pp 1-57 (2013); J. Reedijk and K. Poepplmeier,
 Eds. (S. Alvarez, Vol. 9, Ed.)
<http://dx.doi.org/10.1016/B978-0-08-097774-4.00901-3>
- (426) Y. Wang, D. Janardanan, D. Usharani, K. Han, L. Que, Jr., S. Shaik
 “Nonheme Iron Oxidant Formed in the Presence of H₂O₂ and Acetic Acid is the Cyclic Ferric Peracetate
 Complex, Not a Perferryloxo Complex”
ACS. Catal. **3**, 1334-1341 (2013)
<https://doi.org/10.1021/cs400134g>
- (427) D. Usharani, D. Janardanan, C. Li, S. Shaik
 “A Theory for Bioinorganic Chemical Reactivity of Oxometal Complexes and Analogous Oxidants: The
 Exchange and Orbital-Selection Rules “
Acc. Chem. Res. **46**, 471-482 (2013)
<https://doi.org/10.1021/ar300204y>
- (428) S. Shaik, H.S. Rzepa, R. Hoffmann
 “One Molecule, Two Atoms, Three Views, Four Bonds?”
Angew. Chem. Int. Ed. **52**, 3020-3033 (2013)
<https://doi.org/10.1002/anie.201208206>
- (429) D. Danovich, A. Bino, S. Shaik
 “Formation of Carbon-Carbon Triply Bonded Molecules from Two Free Carbyne Radicals via a Conical
 Intersection”
J. Phys. Chem. Lett. **4**, 58-64 (2013)
<https://doi.org/10.1021/jz3016765>
- (430) J. Song, Z. Chen, S. Shaik, W. Wu
 “An Efficient Algorithm for Complete Active Space Valence Bond Self-Consistent Field Calculations”
J. Comput. Chem. **34**, 38-48 (2013).
<https://doi.org/10.1002/jcc.23103>
- (431) G. Zhang, K. Chen, H. Chen, J. Yao, S. Shaik
 “What Factors Control O₂ Binding and Release Thermodynamics in Mononuclear Ruthenium Water Oxidation
 Catalysts? A Theoretical Exploration”
Inorg. Chem. **52**, 5088-5096 (2013)
<https://doi.org/10.1021/ic3028644>
- (432) S. Ye, C-Y. Geng, S. Shaik, F. Neese
 “Electronic Structure Analysis of Multistate Reactivity in Transition Metal Catalyzed Reactions: The Case of C-
 H Bond Activation by Non-Heme Iron(IV)-Oxo Cores”
PCCP. **15**, 8017-8030 (2013)
<https://doi.org/10.1039/C3CP00080J>
- (433) C. Li, S. Shaik
 “How do Fluorinated Alkanoic Acids Elicit Cytochrome P450 to Catalyze Methane Hydroxylation? An MD and
 QM/MM Study”

- RSC. Adv.* **3**, 2995-3005 (2013)
<https://doi.org/10.1039/C2RA22294A>
- (434) D. Danovich, S. Shaik, H. Rzepa, R. Hoffmann
 “A Response to the Critical Comments on ‘One Molecule, Two Atoms, Three Views, Four Bonds?’ “
Angew. Chem. Int. Ed. **52**, 5926-5928 (2013).
<https://doi.org/10.1002/anie.201302350>
- (435) B. Wang, C. Li, K.-B. Cho, W. Nam, S. Shaik
 “The Fe^{III}(H₂O₂) Complex as a Highly Efficient Oxidant in Sulfoxidation Reactions: Revival of an Underrated Oxidant in Cytochrome P450”
J. Chem. Theor. Comput. **9**, 2519-2525 (2013)
<https://doi.org/10.1021/ct400190f>
- (436) Y.M. Kim, K.-B. Cho, J. Cho, B. Wang, C. Li, S. Shaik, W. Nam
 “A Mononuclear Non-Heme High-Spin Iron(III)-Hydroperoxo Complex as an Active Oxidant in Sulfoxidation Reactions”.
J. Am. Chem. Soc. **135**, 8838-8841 (2013)
<https://doi.org/10.1021/ja404152q>
- (437) S. Shaik
 “An Anatomy of the Two-State Reactivity Concept: Personal Reminiscences in Memoriam of Detlef Schroeder”.
Int. J. Mass Spectrom., **354-355**, 5-14 (2013).
<http://dx.doi.org/10.1016/j.ijms.2013.05.032>
- (438) D. Usharani, D. C. Lacy, A. S. Borovik, S. Shaik, Dichotomous Hydrogen Atom Transfer vs. Proton-Coupled Electron Transfer During Activation of X-H Bonds (X=C, N, O) by Nonheme Iron-Oxo Complexes of Variable Basicity,
J. Am. Chem. Soc. **135**, 17090-17104 (2013)
<https://doi.org/10.1021/ja408073m>
- (439) G. Dong, S. Shaik, W.Z. Lai
 “Oxygen Activation by Homoprotocatechuate 2,3-dioxygenase: A QM/MM Study Reveals the Key Intermediates in the Activation Cycle”.
Chem. Sci. **4**, 3624-3635 (2013)
<https://doi.org/10.1039/C3SC51147B>

2014

- (440) CHAPTER
 D. Danovich, S. Shaik,
 “Bound Triplet Pairs in the Highest Spin States of Monovalent Metal Clusters”
 Pages 149-174 in: *The Chemical Bond*, Vol. 2. G. Frenking and S. Shaik, eds. Wiley-VCH, Weinheim, Germany, 2014
<https://doi.org/10.1002/9783527664658.ch6>
- (441) CHAPTER
 S. Shaik, D. Danovich, W. Wu, P.C. Hiberty
 “The Valence Bond Perspective of the Chemical Bond”
 Pages 159-196 in: *The Chemical Bond*, Vol. 1. G. Frenking and S. Shaik, eds. Wiley-VCH, Weinheim, Germany, 2014
<https://doi.org/10.1002/9783527664696.ch5>
- (442) CHAPTER
 P.C. Hiberty, S. Shaik
 “Bridging Cultures”
 Pages 69-90 in: *The Chemical Bond*, Vol. 1. G. Frenking and S. Shaik, eds. Wiley-VCH, Weinheim, Germany, 2014
<https://doi.org/10.1002/9783527664696.ch2>
- (443) S. Shaik
 Book Review on: “What is Chemistry?” (by Peter Atkins)
Angew. Chem. Int. Ed. **53**, 5004-5005 (2014) <https://doi.org/10.1002/anie.201400523>
- (444) Y. Yang, H. Zhang, D. Usharani, W. Bu, S. Im, M. Tarasev, F. Rwere, N.M. Pearl, J. Meagher, C. Sun, J. Stuckey, S. Shaik, L. Waskell
 “Structural and Functional Characterization of a Cytochrom P450 2B4 F429H Mutant with an Axial Thiolate-Histidine Hydrogen Bond.”
Biochemistry, **53**, 5080-5091 (2014)

- (445) <https://doi.org/10.1021/bi5003794>
S. Shaik, H. Chen, U. Dandamudi, W. Thiel
“QM/MM Studies of Structure and Reactivity of Cytochrome P450 Enzymes: Methodology and Selected Applications.”
Pages 133-178, in “Drug metabolism Predictions”, Ed. J. Kirchmair
Wiley VCH, Weinheim, 2014
<https://doi.org/10.1002/9783527673261.ch06>
- (446) U. Dandamudi, W.Z. Lai, C. Li, H. Chen, D. Danovich, S. Shaik
“A Tutorial for Understanding Chemical Reactivity Through the Valence Bond Approach”
Chem. Soc. Rev. **43**, 4968-4988 (2014)
<https://doi.org/10.1039/C4CS00043A>
- (447) D. Danovich, S. Shaik
“Bonding with Parallel Spins: High-Spin Clusters of Monovalent Metal Atoms”
Acc. Chem. Res. **47**, 417-426 (2014).
<https://doi.org/10.1021/ar4001422>
- (448) W. Wu, H. Zhang, B. Braida, S. Shaik, P.C. Hiberty.
“The V State of Ethylene: Valence Bond Theory Takes Up the Challenge”.
Theor. Chem. Acc. **133**, 1441 (pp. 1-13) (2014)
<https://doi.org/10.1007/s00214-013-1441-x>
- (449) D. Danovich, P.C. Hiberty, W. Wu, H.S. Rzepa, S. Shaik
“The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum”
Chem. Eur. J., **20**, 6220-6232 (2014)
<https://doi.org/10.1002/chem.201400356>
- (450) W. N. Oloo, K.K. Meier, Y. Wang, S. Shaik, E. Münck, L. Que, Jr.
“Identification of a Low-Spin Matrix Acylperoxoiron(III) Intermediate in Bio-Inspired Non-heme Iron-Catalysed Oxidations”
Nature Communications, **5**, 3046, (2014)
<https://doi.org/10.1038/ncomms4046>
- (451) H. Zhang, D. Danovich, W. Wu, B. Braida, P.C. Hiberty, S. Shaik
“Charge-Shift Bonding Emerges as a Distinct Electron-Pair Bonding Family from Both Valence Bond and Molecular Orbital Theories”.
J. Chem. Theor. Comput. **10**, 2410-2418 (2014)
<https://doi.org/10.1021/ct500367s>
- (452) CHAPTER
S. Shaik, G. Frenking
Preface to “The Chemical Bond”, Vol. 1, pp. XIII-XXI.
Wiley-VCH, Weinheim, Germany, 2014
<https://doi.org/10.1002/9783527664696.fmatter>
- (453) CHAPTER
G. Frenking, S. Shaik
Preface to “The Chemical Bond”, Vol. 2, pp. XV-XVIII.
Wiley-VCH, Weinheim, Germany, 2014.
- (454) C. Wang, D. Danovich, Y. Mo, S. Shaik
“On the Nature of the Halogen-Bond”
J. Chem. Theor. Comput. **10**, 3726-3737 (2014)
<https://doi.org/10.1021/ct500422t>
- (455) B. Wang, D. Usharani, C. Li, S. Shaik
“Theory Uncovers an Unusual Mechanism of DNA Repair of a Lesioned Adenine by AlkB Enzymes”
J. Am. Chem. Soc. **136**, 13895-13901 (2014).
<https://doi.org/10.1021/ja507934g>
Spotlighted in *J. Am. Chem. Soc.* 2014, **136**, 14321-14322
- (456) R. Kang, K. Chen, J. Yao, S. Shaik, H. Chen
“Probing Ligand Effects on O-O Bond Formation of Ru-Catalyzed Water Oxidation: A Computational Survey”
Inorg. Chem. **53**, 7130-7136 (2014)
<https://doi.org/10.1021/ic500008c>
- (457) K.B. Cho, J. Cho, S. Shaik, W. Nam
“Investigating Superoxide Transfer Through a μ -1,2-O₂ Bridge between Nonheme Ni^{III}-Peroxo and Mn^{II} Species by DFT Methods to Bridge Theoretical and Experimental Views”

- J. Phys. Chem. Lett.* **5**, 2437-2442 (2014)
<https://doi.org/10.1021/jz501193k>
- (458) P. Anderson, A. Petit, J. Ho, M.P. Mitoraj, M.L. Coote, D. Danovich, S. Shaik, B. Barida, D.H. Ess
 “Protonated Alcohols are Examples of Complete Charge-Shift Bonds”
J. Org. Chem. **79**, 9998-10001 (2014)
<https://doi.org/10.1021/jo501549q>
- (459) EDITING
 G. Frenking, S. Shaik, Editors
 “The Chemical Bond”, Vol. 1
 Wiley-VCH, Mannheim, Germany 2014.
- (460) EDITING
 G. Frenking, S. Shaik, Editors
 “The Chemical Bond”, Vol. 2
 Wiley-VCH, Mannheim, Germany 2014.
- 2015**
- (461) D. Mandal, R. Ramanan, D. Usharani, D. Janardanan, B. Wang, S. Shaik
 “How Does Tunneling Contribute to Counterintuitive C-H Abstraction Reactivity of Nonheme Fe(IV)O Oxidants with Alkanes?”
J. Am. Chem. Soc. **137**, 722–733 (2015)
<https://doi.org/10.1021/ja509465w>
- (462) Y.H. Kwon, B.K. Mai, Y.-M. Lee, S.N. Dhuri, D. Mandal, K.-B. Cho, Y. Kim, S. Shaik, W. Nam,
 “Determination of Spin Inversion Probability, H-Tunneling Correction, and Regioselectivity in the Two-State Reactivity of Nonheme Iron(IV)-Oxo Complexes”
J. Phys. Chem. Lett. **6**, 1472-1476 (2015)
<https://doi.org/10.1021/acs.jpcllett.5b00527>
- (463) B. Wang, C. Li, K.D. Dubey, S. Shaik
 “Quantum Mechanical/Molecular Mechanical Calculated Reactivity Networks Reveal How Cytochrome P450_{cam} and Its T252A Mutant Select Their Oxidation Pathways”
J. Am. Chem. Soc. **137**, 7379-7390 (2015)
<https://doi.org/10.1021/jacs.5b02800>
- (464) C. Wang, Y. Mo, J.P. Wagner, P.R. Schreiner, E.D. Jemmis, D. Danovich, S. Shaik
 “The Self-Association of Graphane Is Driven by London Dispersion and Enhanced by Orbital Interactions”
J. Chem. Theor. Comput. **11**, 1621-1630 (2015)
<https://doi.org/10.1021/acs.jctc.5b00075>
- (465) S. Shaik, S. Alvarez,
 “Reply to ‘Entropic Factors Also Contribute to the High Melting of Polyhedral Alkanes’”
Nature Chem. **7**, 89-90 (2015)
<https://doi.org/10.1038/nchem.2147>
- (466) P.C. Hiberty, D. Danovich, S. Shaik
 “Comment on ‘Rabbit-Ears Hybrids, VSPER Sterics, and Other Orbital Anachronism’. A Reply to a Criticism”
Chem. Educ. Res. Pract. **16**, 689-693 (2015)
<https://doi.org/10.1039/C4RP00245H>
- (467) S. Shaik
 “A Tale of Two Mounts: The History of Chemistry at the Hebrew University of Jerusalem”
Isr. J. Chem. **55**, 781-825 (2015)
<https://doi.org/10.1002/ijch.201510006>
- (468) S.N. Dhuri, K.B. Cho, Y.-M. Lee, S.Y. Shin, J.H. Kim, D. Mandal, S. Shaik, W. Nam
 “Interplay of Experiment and Theory in Elucidating Mechanisms of Oxidation Reactions by a Nonheme Ru^{IV}O Complex.”
J. Am. Chem. Soc. **137**, 8623-8632 (2015)
<https://doi.org/10.1021/jacs.5b04787>
- (469) B. Wang, Z. Cao, D.A. Sharon, S. Shaik,
 “Computations Reveal a Rich Mechanistic Variation of Demethylation of N-Methylated DNA/RNA Nucleotides by FTO”
ACS. Catal. **5**, 7077-7090 (2015)
<https://doi.org/10.1021/acscatal.5b01867>
- (470) J. England, J. Prakash, M.A. Cranswick, D. Mandal, Y. Guo, E. Münck, S. Shaik, L. Que Jr.

- “Oxoiron(IV) Complex of the Ethylene-Bridged Dialkylcyclam Ligand Me₂EBC”
Inorg. Chem. **54**, 7828-7839 (2015)
<https://doi.org/10.1021/acs.inorgchem.5b00861>
- (471) S. Shaik, D. Danovich, P.C. Hiberty.
 “Response to the Comment on “The Nature of the Fourth Bond in the Ground State of C₂: The Quadruple Bond Conundrum.”
Chem. Eur. J. **21**, 17127-17128 (2015)
<https://doi.org/10.1002/chem.201503882>
- (472) S. Shaik, M. Karni, D. Danovich, Y. Apeloig.
 “The Lise Meitner-Minerva Center for Computational Quantum Chemistry: 18 Years of Israeli-German Collaboration”
Isr. J. chem. **55**, 1167-1176 (2015)
<https://doi.org/10.1002/ijch.201500079>
- (473) T. Zeng, D. Danovich, S. Shaik, N. Ananth, R. Hoffmann
 “Tuning the Ground State Symmetry of Acetylenyl Radicals”
ACS Central Science, **1**, 270-278 (2015)
<https://doi.org/10.1021/acscentsci.5b00187>

2016

- (474) CHAPTER
 S. Shaik, D. Danovich, B. Braida, W. Wu, P.C. Hiberty
 “New Landscape of Electron-Pair Bonding: Covalent, Ionic and Charge-Shift Bonds”
Structure and Bonding (The Chemical Bond II – 100 Years Old and Getting Stronger), **170**, 169-212 (2016)
https://doi.org/10.1007/430_2015_179
- (475) K. D. Dubey, B. Wang, S. Shaik
 “Molecular Dynamics and QM/MM Calculations Predict the Substrate-Induced Gating of Cytochrome P450 BM3 and the Regio- and Stereoselectivity of Fatty Acid Hydroxylation”
J. Am. Chem. Soc. **138**, 837-845 (2016)
<https://doi.org/10.1021/jacs.5b08737>
- (476) D. Danovich, S. Shaik
 “On the Nature of Bonding in Parallel Spins in Monovalent Metal Clusters”
Annu. Rev. Phys. Chem. **67**, 419-439 (2016)
<https://doi.org/10.1146/annurev-physchem-040215-112324>
- (477) K.B. Cho, H. Hirao, S. Shaik, W. Nam
 “To Rebound or Dissociate? This is the Mechanistic Question in C-H Hydroxylation by Heme and Nonheme Metal-Oxo Complexes”
Chem. Soc. Rev. (Tutorial), **45**, 1197-1210 (2016)
<https://doi.org/10.1039/C5CS00566C>
- (478) D. Mandal, S. Shaik
 “Interplay of Tunneling, Two-state Reactivity and Bell-Evans-Polanyi Effects in C-H Activation by Nonheme Fe(IV)O Oxidants”.
J. Am. Chem. Soc. **138**, 2094-2097 (2016)
<https://doi.org/10.1021/jacs.5b12077>
- (479) J. Huang, C. Li, B. Wang, D.A. Sharon, W. Wu, S. Shaik
 “Selective Chlorination of Substrates by Halogenase SyrB2 is controlled by the Protein According to Combined Quantum Mechanics/Molecular Mechanics and Molecular Dynamics Study”.
ACS Catal. **6**, 2694-2704 (2016)
<https://doi.org/10.1021/acscatal.5b02825>
- (480) S. Shaik, D. Danovich, B. Braida, P. C. Hiberty
 “The Quadruple Bonding in C₂ Reproduces the Properties of the Molecule”.
Chem. Eur. J. **22**, 4116-4128 (2016)
<https://doi.org/10.1002/chem.201600011>
- (481) D. Mallick, S. Shaik
 “Theory Reveals the Unusual Non-Rebound Mechanisms Responsible for the Distinct Reactivities of O=Mn^{IV}=O and [HO-Mn^{IV}-OH]²⁺ Towards C-H Bond Activation”.
ACS Catal. **6**, 2877-2888 (2016)
<https://doi.org/10.1021/acscatal.6b00085>

- (482) C. Wang, L. Guan, D. Danovich, S. Shaik, Y. Mo
 “The Origins of the Directionality of Non-Covalent Intermolecular Interactions”
J. Comput. Chem. **37**, 34-45 (2016)
<https://doi.org/10.1002/jcc.23946>
- (483) **CHAPTER**
 D. Usharani, B. Wang, D. A. Sharon, S. Shaik
 “Principles and Prospects of State-States Reactivity in Chemistry and Bioinorganic Chemistry”, in *Spin-States in Biochemistry and inorganic Chemistry: Influence on Structure and Reactivity*, M. Swart and M. Costas, Eds.
 Wiley & Sons Ltd., New York, pp. 131-156, (2016)
<https://doi.org/10.1002/9781118898277.ch7>
- (484) R. Ramanan, K. D. Dubey, B. Wang, D. Mandal, S. Shaik
 “Emergence of Function in P450-Proteins: A Combined Quantum Mechanical/Molecular Mechanical and Molecular Dynamics Study of the Reactive Species in the H₂O₂-Dependent Cytochrome P450_{SP α} and Its Regio- and Enantioselective Hydroxylation of Fatty Acids”.
J. Am. Chem. Soc. **138**, 6786-6797 (2016).
<https://doi.org/10.1021/jacs.6b01716>
Issue Cover, and **Spotlighted** (JACS, **138**, 6689 (2016))
- (485) B. Wang, J. Lu, K. D. Dubey, G. Dong, W.Z. Lai, S. Shaik,
 “How Do Enzymes Utilize Reactive OH Radicals? Lessons from Non-Heme HppE and Fenton Systems”.
J. Am. Chem. Soc. **138**, 8489-8496 (2016)
<https://doi.org/10.1021/jacs.6b03555>
- (486) Y. Sun, H. Tang, K. Chen, L. Hu, J. Yao, S. Shaik, H. Chen.
 “Two-State reactivity in Low-Valent Iron-Mediated C-H Activation and the Implications for other First-Row Transition Metals”.
J. Am. Chem. Soc. **138**, 3715-3730 (2016)
<https://doi.org/10.1021/jacs.5b12150>
- (487) D. A. Sharon, D. Mallick, B. Wang, S. Shaik
 “Computational Sheds Insights into Iron Porphyrin Carbenes’ Electronic Structure, Formation, and N-H Insertion Reactivity”.
J. Am. Chem. Soc. **138**, 9597-9610 (2016)
<https://doi.org/10.1021/jacs.6b04636>
- (488) S. Shaik, D. Mandal, R. Ramanan
 “Oriented Electric Fields as Future Smart Reagents in Chemistry”
Nature Chem. **8**, 1091-1098 (2016).
<https://doi.org/10.1038/nchem.2651>
- (489) J. Li, S. Zhou, J. Zhang, M. Schlangen, T. Weiske, D. Usharani, S. Shaik, H. Schwarz
 “Electronic Origins of the Variable Efficiency of Room-Temperature Methane Activation by Homo- and Heteronuclear Cluster Oxide Cations [XYO₂]⁺ (X, Y = Al, Si, Mg): Competition between Proton-Coupled Electron Transfer and Hydrogen-Atom Transfer”
J. Am. Chem. Soc. **138**, 7973-7981 (2016)
<https://doi.org/10.1021/jacs.6b03798>
- (490) S. Shaik, D. Danovich, B. Braida, P. C. Hiberty
 “A Response to a Comment on: ‘The Quadruple Bonding in C₂ Reproduces the Properties of the Molecule”
Chem. Eur. J. **22**, 18977-18980, (2016)
<https://doi.org/10.1002/chem.201602840>
- (491) J. Li, S. Zhou, J. Zhang, M. Schlangen, D. Usharani, S. Shaik, H. Schwarz
 “Mechanistic Variants in Gas-Phase Metal-Oxide Mediated Activation of Methane at Ambient Conditions”
J. Am. Chem. Soc. **138**, 11368-11377 (2016). **Spotlighted:** *J. Am. Chem. Soc.* **2016**, *138*,
<https://doi.org/10.1021/jacs.1026b09412>
- (492) “Catching Up with Sason Shaik”
 Posted by Marshall Brennan in *thescepticalChymist - Nature Chemistry Blog*
 25th November 2016 in “Reactions”.
- (493) **BOOK**
 S. Shaik
 With contributions by R. Ben-Knaz, U. Dandamudi and D.A. Sharon.
 Foreword by: R. Hoffmann.
 “Chemistry as a Game of Molecular Construction: The Bond-Click Way”
 pp. 1-546.
 John Wiley & Sone, Inc. Hoboken, New Jersey, 2016

This book is among the best-selling Chemistry eBooks at all times:

<https://bookauthority.org/books/best-selling-chemistry-ebooks>

*A top review is displayed below – underneath the list of publications:

2017

- (494) S. Radenkovic, D. Danovich, S. Shaik, P. C. Hiberty, B. Braida,
“The Nature of Bonding in Metal-Metal Singly Bonded Coinage Metal Dimers”.
Comput. & Theor. Chem. **1116**, 195-201 (2017)
<https://doi.org/10.1016/j.comptc.2017.02.013>
- (495) S. Shaik, P.C. Hiberty
“Valence Bond Theory in Chemistry”
An invited chapter in: Theoretical and Computational Advances: From Atoms to Molecules to Materials”, (the Mihir Roychoudhury Festschrift), D. Kumar, Ed., pp. 1-20, Lucknow (U. P.) India, (2017).
- (496) D. Mallick, S. Shaik
“Kinetic Isotope Effect Probes the Reactive-Spin State, as Well as the Geometric Feature and Constitution of the Transition State During H-Abstraction by Heme Compound II Complexes”.
J. Am. Chem. Soc. **139**, 11451-11459 (2017)
<https://doi.org/10.1021/jacs.7b11300>
- (497) C. Wang, D. Danovich S. Shaik, Y. Mo
“Halogen Bonds in Novel Polyhalogen Monoanions”
Chem. Eur. J. **23**, 8719-8728 (2017)
<https://doi.org/10.1002/chem.201701116>
- (498) J. Bigelow, J. England, J. E. M. N. Klein, E. R. Farquhar, J. R. Frisch, M. Martinho, D. Mandal, E. Münck, S. Shaik, L. Que, Jr.
“Oxoiron(IV) Tetramethylcycloam Complexes with Axial Carboxylate Ligands: Effect of Tethering the Carboxylate on Reactivity”
Inorg. Chem. **56**, 3287-3301 (2017)
<https://doi.org/10.1021/acs.inorgchem.6b02659>
- (499) J. Gu, W. Wu, D. Danovich, R. Hoffmann, T. Yuta, S. Shaik
“Valence Bond Theory Reveals the Hidden Delocalized Diradical Character of Polyenes”
J. Am. Chem. Soc. **139**, 9302-9316 (2017)
<https://doi.org/10.1021/jacs.7b04410>
Spotlight: “Duality of Polyene’s Electronic Structure”, *J. Am. Chem. Soc.* **139**, 9089-9089 (2017).
- (500) M. Kaupp, D. Danovich, S. Shaik
“Chemistry is About Energy and Its Changes: A Critique of Bond-Length/Bond-Strength Correlations”
Coord. Chem. Rev **344**, 355-362 (2017)
<https://doi.org/10.1016/j.ccr.2017.03.002>
- (501) A. Li, B. Wang, A. Ilie, K. D. Dubey, G. Bange, I. V. Korendovych, S. Shaik, M. T. Reetz ,
“A Redox-Mediated Kemp Eliminate”.
Nature Communications (NCOMMS), **8**:14876 (2017)
<https://doi.org/10.1038/ncomms14876>
- (502) K. D. Dubey, B. Wang, M. Vajpai, S. Shaik
“MD Simulations and QM/MM Calculations Show that Single-Site Mutations of Cytochrome P450 BM3 Alter the Active Site’s Complexity and the Chemoselectivity of Oxidation Without Changing the Active Species”.
Chem. Sci., **8**, 5335 – 5344 (2017)
<https://doi.org/10.1039/C7SC01932G>
- (503) K.-B. Cho, N.Y. Lee, D. Mandal, S. H. Bae, M. S. Seo, Y. M. Lee, S. Shaik, W. Nam
“Structure and Spin-State of Nonheme Fe^{IV}O Complexes Depending on Temperature: Predictive insights from DFT Calculations and Experiments”.
Chem. Sci. **8**, 5460-5467 (2017)
<https://doi.org/10.1039/C7SC01738C>
- (504) S. Shaik, D. Danovich, P. C. Hiberty
“To Hybridize or Not to Hybridize? This is the Dilemma”
Comput. & Theor. Chem. **1116**, 242-249 (2017)
<https://doi.org/10.1016/j.comptc.2017.01.017>
- (505) B. Wang, S. Shaik
“QM/MM Calculations Reveal that the Nickel-Pincer Complex in Lactate Racemase Is an Electron-Relay Sink that Catalyzes the Process via Proton-Coupled Electron-Transfer”

- Angew. Chem. Int.* **56**, 10098-10102 (2017)
<https://doi.org/10.1002/anie.201612065>
- (506) S. Shaik
 “A Personal Story On a Renaissance in Valence Bond Theory: A Theory Coming of Age!”
Comput. & Theor. Chem. **1116**, 2-31 (2017)
<https://doi.org/10.1016/j.comptc.2017.02.011>
- (507) C. Geng, J. Li, T. Weiske, M. Schlangen, S. Shaik, H. Schwarz
 “Electrostatic and Charge-Induced Methane Activation by a Concerted Double C-H Bond Insertion”
J. Am. Chem. Soc. **139**, 1684-1689 (2017)
<https://doi.org/10.1021/jacs.6b12514>
- (508) C. Wang, D. Danovich, S. Shaik, Y. Mo
 “A Unified Theory for the Blue- and Red-Shifting Phenomena in Hydrogen and Halogen Bonds”
J. Chem. Theor. Comput. **13**, 1626-1637 (2017)
<https://doi.org/10.1021/acs.jctc.6b01133>
- (509) L. Yue, J. Li, S. Shodong, X. Sun, M. Schlangen, S. Shaik, H. Schwarz
 “Control of Product Distribution and Mechanism by Ligation and Electric Field in the Thermal Methane Activation”
Angew. Chem. Int. Ed. **56**, 10219-10223 (2017).
<https://doi.org/10.1002/anie.201703485>
Highlighted: Very Important Paper (VIP) & Selected for a Journal Cover
- (510) J.E.M.N. Klein, D. Mandal, W.-M. Ching, D. Mallick, L. Que, Jr., S. Shaik
 “The Privileged Role of Thiolate as the Axial Ligand in HAT Reactions by Oxoiron(IV) Complexes in Shaping the Potential Energy Surface and Inducing Significant H-Atom Tunneling”,
J. Am. Chem. Soc. **139**, 18705-18713 (2017)
<https://doi.org/10.1021/jacs.7b11300>
- (511) H. Schwarz, S. Shaik, J. Li
 “Electronic Effect on Room-Temperature, Gas-Phase C-H Activation by Cluster Oxides and Metal Carbides: The Methane Challenge”
J. Am. Chem. Soc. **139**, 17201-17212 (2017)
 A Perspective
<https://doi.org/10.1021/jacs.7b10139>

2018

- (512) CHAPTER
 S. Shaik
 “Bonds and Intermolecular Interactions - The Return of Cohesion to Chemistry”, in:
 “Intermolecular interactions in Crystals: Fundamentals of Crystal Engineering”, J. J. Novoa, Ed., The Royal Society of Chemistry, London. Chapter 1, 3-68 (2018)
- (513) R. Ramanan, D. Danovich, D. Mandal, S. Shaik
 “Catalysis of Methyl Transfer Reactions by Oriented external Electric Fields: Are Gold Thiolate Linkers Innocent?”
J. Am. Chem. Soc. **140**, 4354-4362 (2018)
<https://doi.org/10.1021/jacs.8b00192>
- (514) D. Mandal, D. Mallick, S. Shaik
 “KIE Determination Probes the Spin of the Transition State, its Stereochemistry, and Ligand Sphere in H-Abstraction Reactions of Oxoiron(IV) Complexes”
Acc. Chem. Res. **51**, 107-117 (2018).
<https://doi.org/10.1021/acs.accounts.7b00442>
- (515) D. Danovich, C. Foroutan-Nejad, P. C. Hiberty, S. Shaik
 “Nature of the Three-Electron Bond”
J. Phys. Chem. A. **122**, 1873-1885 (2018)
<https://doi.org/10.1021/acs.jpca.7b11919>
- (516) C. Wang, Y. Fu, L. Zhang, D. Danovich, S. Shaik, Y. Mo
 “Hydrogen- and Halogen-Bonds Between Ions of Like Charges: Are They Anti-Electrostatic in Nature?”
J. Comput. Chem. **39**, 481-487 (2018)
<https://doi.org/10.1002/jcc.25068>
- (517) K. D. Dubey, S. Shaik

- “Choreography of the Reductase and P450_{BM3} Domains Towards Electron Transfer Is Instigated by the Substrate”
J. Am. Chem. Soc. **140**, 683-690 (2018)
<https://doi.org/10.1021/jacs.7b10072>
- (518) S. Shaik, R. Ramanan, D. Danovich, D. Mandal
 “Structure and Reactivity/Selectivity Control by Oriented-External Electric Fields”
Chem. Soc. Rev. (Tutorial). **47**, 5125-5145 (2018)
<https://doi.org/10.1039/C8CS00354H>
- (519) B. Wang, E.M. Johnston, P. Li, S. Shaik, G.J. Davies, P.H. Walton, C. Rovira
 “QM/MM Studies into the H₂O₂-Dependent Activity of Lytic Polysaccharid Monooxygenases: Evidence for the Formation of a Caged Hydroxyl Intermediate”.
ACS. Catal. **8**, 1346-1351 (2018)
<https://doi.org/10.1021/acscatal.7b03888>
- (520) S. Shaik
 “The Institute of Chemistry in the Hebrew University of Jerusalem: The Pioneer and Godfather of All Chemistry in Israel”. [in Hebrew]
 The Israeli Chemistry Teachers Magazine, 70 Years of Chemistry in Israel, 12-16 (2018).
- (521) Z. Wang, D. Danovich, R. Ramanan, S. Shaik
 “Oriented-External Electric Fields Create Absolute Enantioselectivity in Diels-Alder Reactions: The Importance of the Molecular Dipole Moment”
J. Am. Chem. Soc. **140**, 13350-13359 (2018)
<https://doi.org/10.1021/jacs.8b08233>
- (522) C. Wei, D. Danovich, S. Shaik, W. Wu, Y. Mo
 “Attraction between Electrophilic Caps: A Counterintuitive Case of Non-Covalent Interactions”.
J. Comput. Chem. **40**, 1015-1022 (2018)
<https://doi.org/10.1002/jcc.25566>
- (523) C. Geng, J. Li, M. Schlangen, S. Shaik, X. Sun, N. Wang, T. Weiske, L. Yue, S. Zhou, H. Schwarz
 “Oriented External Electric Fields as a Mimic for Probing the Role of Metal Ions and Their Ligands in the Thermal Gas-phase Activation of Methane.”
 A Frontier Article
Dalton Trans. **47**, 15271-15277 (2018)
<https://doi.org/10.1039/C8DT03048K>
- 2019**
- (524) K. D. Dubey, S. Shaik
 “Cytochrome P450 - The Wonderful Nano-Machine Revealed Through Dynamic Simulation of the Catalytic Cycle”.
Acc. Chem. Res. **52**, 389-399 (2019)
<https://doi.org/10.1021/acs.accounts.8b00467>
- (525) J. Gu, W. Wu, T. Stuyver, D. Danovich, R. Hoffmann, Y. Tsuji, S. Shaik
 “Cross Conjugation in Polyenes and Related Hydrocarbons: What Can be Learned from Valence Bond Theory on Single-Molecular Conductance?”
J. Am. Chem. Soc. **141**, 6030-6047 (2019)
<https://doi.org/10.1021/jacs.9b01420>
- (526) D. G. Truhlar, S. Shaik, M. S. Gordon, D. Danovich, P. C. Hiberty
 “Orbitals and Interpretation of Photoelectron Spectroscopy Experiments”
Angew. Chem. Int. Ed. **58**, 12332-12338 (2019)
<https://doi.org/10.1002/anie.201904609>
- (527) C. Geng, T. Weiske, J. Li, S. Shaik, H. Schwarz
 “On the Intrinsic Reactivity of Diatomic 3d Transition-Metal Carbides in the Thermal Activation of Methane: Striking Electronic Structure Effects”.
J. Am. Chem. Soc. **141**, 599-610 (2019)
<https://doi.org/10.1021/jacs.8b11739>
- (528) S. Shaik
 “Helmut Schwarz – A Story of Science and Friendship”
Int. J. Mass Spectrom. **435**, 151-162 (2019)
<https://doi.org/10.1016/j.ijms.2018.10.015>
- (529) C. Wang, D. Danovich, H. Chen, S. Shaik

- “Oriented External Electric Fields – Tweezers and Catalysts for Reactivity in Halogen-Bond Complexes”.
J. Am. Chem. Soc. **141**, 7122-7136 (2019)
<https://doi.org/10.1021/jacs.9b02174>
- (530) P. C. Hiberty, D. Danovich, S. Shaik
 “Comment on “Decoding Real Space Description in Valence Bond Language”
Phys. Chem. Chem. Phys. **21**, 8170-8174 (2019)
<https://doi.org/10.1039/c8cp07225f>
- (531) S. Hao, B. Wang, S. Shaik
 “QM/MM Studies of CYP11A1-Catalyzed Biosynthesis of Pregnenolone from Cholesterol Reveal a C-C Bond
 Cleavage Reaction that Occurs by a Cpd I-Mediated Electron Transfer”.
J. Am. Chem. Soc. **141**, 20079-20088 (2019)
<https://doi.org/10.1021/jacs.9b08561>
- (532) T. Stuyver, D. Danovich, J. Jyothish, S. Shaik
 “External Electric Field Effects on Chemical Structure and Reactivity”
WIREs Comput Mol Sci. **10**, 1-22 (2019); e1438
<https://doi.org/10.1002/wcms.1438>
- (533) T. Stuyver, D. Danovich, S. Shaik
 “Insights into the Trends in the Acidity of Organic and Inorganic Compounds: A Valence Bond Perspective”
J. Phys. Chem. A. **123**, 1851-1860 (2019)
<https://doi.org/10.1021/acs.jpca.9b01095>
- (534) S. Shaik, E. Cremades, S. Alvarez
 “The Periodic-Table A Universal Icon: Its Birth 150 Years Ago, and Its Popularization Through Literature,
 Art and Music”.
Angew. Chem. Int. Ed. **58**, 13194-13206 (2019)
<https://doi.org/10.1002/anie.201904584>
- (535) B. Wang, X. Cao, C. Rovira, S. Shaik
 “Fenton-Derived OH Radical Enable the MPnS Enzyme to Convert 2-Hydroxyphosphonate to
 Methylphosphonate: Insights from Ab Initio QM/MM MD Simulations”.
J. Am. Chem. Soc. **141**, 9284-9291 (2019)
<https://doi.org/10.1021/jacs.9b02659>
- (536) T. Stuyver, D. Danovich, F. De Proft, S. Shaik,
 “Electrophilic Aromatic Substitution Reactions: Mechanistic Landscape, Electrostatic and Electric-Field
 Control of Reaction Rates and Mechanistic Crossovers”
J. Am. Chem. Soc. **141**, 9719-9730 (2019)
<https://doi.org/10.1021/jacs.9b04982>
- (537) T. Stuyver, D. Danovich, S. Shaik
 “Captodative Substitution Enhances the Diradical Character of Compounds, Reduces Aromaticity and Controls
 Single Molecule Conductivity Patterns: A Valence Bond Study”.
J. Phys. Chem. A. **123**, 7133-7141 (2019)
<https://doi.org/10.1021/acs.jpca.9b06096>
- (538) T. Stuyver, J. Huang, D. Mallick, D. Danovich, S. Shaik
 “TITAN: A Code for Modeling and Generating Electric Fields - Features and Applications to Enzymatic
 Reactivity”
J. Comput. Chem. **41**, 74-82 (2019)
<https://doi.org/10.1002/jcc.26072>
- 2020**
- (539) T. Stuyver, R. Ramanan, D. Mallick, S. Shaik
 “Oriented Electric Fields Drive Millionfold H-Abstraction Catalysis Observed for Synthetic Metalloenzyme
 Analogues”.
Angew. Chem. Int. Ed. **59**, 7915-7920 (2020)
<https://doi.org/10.1002/anie.201916592>
- (540) **An Invited Perspective:**
 S. Shaik, D. Danovich, J. Joy, Z. Wang, T. Stuyver
 “Electric-field mediated chemistry: uncovering and exploiting the potential of (oriented) electric fields to exert
 chemical catalysis and reaction control”
J. Am. Chem. Soc. **142**, 12551-12562 (2020)

- <https://doi.org/10.1021/jacs.0c05128>
- (541) S. Shaik, D. Danovich, J. M. Galraith, B. Braida, W. Wu, P. C. Hiberty
“Charge-Shift Bonding: A New and Unique Form of Bonding”
Angew. Chem. Int. Ed. **59**, 984-1001 (2020)
<https://doi.org/10.1002/anie.201910085>
- (542) K. D. Dubey, T. Stuyver, S. Kalita, S. Shaik
“Solvent-Reorganization and Rate-Regulation of a Menshutkin Reaction by Oriented-External Electric Fields are Revealed by Combination of MD and QM/MM Calculations”
J. Am. Chem. Soc. **142**, 9955-9965 (2020)
<https://doi.org/10.1021/jacs.9b13029>
- (543) J. Joy, T. Stuyver, S. Shaik
“Oriented External Electric Fields and Ionic Additives Elicit Catalysis and Mechanistic Cross-Over in Oxidative Addition Reactions”
J. Am. Chem. Soc. **142**, 3836-3850 (2020)
<https://doi.org/10.1021/jacs.9b11507>
- (544) S. Shaik
“Two-State Reactivity: Personal Recounting of Its Conception and Future Prospects”
Isr. J. Chem. **60**, 938-956 (2020)
<http://dx.doi.org/10.1002/ijch.202000002>
- (545) B. Braida, S. Shaik, W. Wu, P.C. Hiberty
“Comment on “The ‘Inverted Bond’ Revisited. Analysis of ‘in silico’ Models of [1.1.1]Propellane Using Orbital Forces”
Chemistry- Eur. J. **26**, 6935-6939 (2020)
<https://doi.org/10.1002/chem.201905666>
- (546) J. Lu, B. Wang, S. Shaik, W.Z. Lai
“QM/MM Calculations Reveal Important Role of α -Heteroatom Substituents in Controlling Selectivity of Mononuclear Nonheme HppE-Catalyzed Reactions”
ACS Catal. **10**, 9521-9532 (2020)
<https://doi.org/10.1021/acscatal.0c01803>
- (547) R. Meir, H. Chen, W. Lai, S. Shaik
“Oriented Electric Fields Accelerate Diels-Alder Reactions and Control the *endo/exo* Selectivity”.
[Original: *ChemPhysChem.* **11**, 301-310 (2010)]
A corrigendum: *ChemPhysChem.* **21**, 1 (2020)
<https://doi.org/10.1002/cphc.201701187>
- (548) T. Stuyver, S. Shaik
“Unifying Conceptual Density Functional and Valence Bond Theories: The Hardness-Softness Conundrum Associated with Protonation Reactions and Uncovering Complementary Reactivity Modes”
J. Am. Chem. Soc. **142**, 20002-20013 (2020).
<https://dx.doi.org/10.1021/jacs.0c09041>
- (549) J. Joy, D. Danovich, M. Kaupp, S. Shaik
“On the Covalent vs. Charge-Shift Nature of the Metal-Metal Bond in Transition Metal Complexes”
J. Am. Chem. Soc. **142**, 12277-12287 (2020)
<https://dx.doi.org/10.1021/jacs.0c03957>
- (550) S. Kalita, S. Shaik, H. Kisan, K.D. Dubey
“A Paradigm Shift in the Catalytic Cycle of P450 – The Preparatory Choreography During O₂ Binding, and Origins of the Necessity for Two Protonation Pathways”
ACS Catal., **10**, 9521-9532 (2020)
<https://doi.org/10.1021/acscatal.0c02775>
- (551) T. Stuyver, F. De Proft, P. Geerlings, S. Shaik
“How Do Local Reactivity Descriptors Shape the Potential Energy Surface Associated with Chemical Reactions? The Valence Bond Delocalization Perspective”
J. Am. Chem. Soc. **142**, 10102-10113 (2020)
<https://doi.org/10.1021/jacs.0c02390>
- (552) S. Shaik, P.C. Hiberty,
“A New Type of Bond: Charge Shift Bonds”
Adv. Sci. News, July 3, (2020)
A newly discovered class of fundamental bonding interactions is changing our understanding of chemistry
<https://www.advancedsciencenews.com/a-new-type-of-bond-charge-shift-bonds/>

- (553) Corrigendum : D.G. Truhlar, P.C. Hiberty, S. Shaik, M.S. Gordon, D. Danovich, [Original: "Orbitals and the Interpretation of Photoelectron Spectroscopy in (e,2e) Ionization Experiments" *Angew. Chem. Int. Ed.* **58**, 12332-12338 (2019)]
Corrigendum, *Angew. Chem. Int. Ed.* **59**, 12574 (2020)
<https://doi.org/10.1002/anie.201904609> .

2021

- (554) CHAPTER [*moved to 2024]
S. Shaik, T. Travis
"The History of Chemistry at Hebrew University of Jerusalem During 1948-1967".
Magness-Press, in press (2021-2023).
Language: Hebrew
- (555) S. Shaik, T. Stuyver,
PREFACE to the EDITED BOOK: "Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry" (2021)
<https://doi.org/10.1039/9781839163043>
- (556) S. Shaik, T. Stuyver
INTRODUCTION to: "Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry", pp 1-11 (2021)
<https://doi.org/10.1039/9781839163043-00001>
- (557) S. Shaik, D. Danovich, K. D. Dubey, T. Stuyver
CHAPTER 2: "The Impact of Electric Fields on Structure and Reactivity"
In: "Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry", pp 12-70
The Royal Society of Chemistry, 2021, pp. 1-421
<https://doi.org/10.1039/9781839163043-00012>
- (558) T. Stuyver, J. Joy, D. Danovich, S. Shaik
CHAPTER 6: Computational Generation and Quantification of Electric Fields and Electrostatics-Mediated Catalyst Optimization"
In: "Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry", pp 195-224.
The Royal Society of Chemistry, 2021, pp. 1-421
<https://doi.org/10.1039/9781839163043-00195>
- (559) S. Shaik, T. Stuyver
CHAPTER 12: Concluding Remarks. pp. 420-421
In: "Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry"
The Royal Society of Chemistry, 2021, pp. 1-421
<https://doi.org/10.1039/9781839163043-00420>
- (560) T. Mondal, S. Shaik, H. Kenttämaa, T. Stuyver
"Modulating the Radical Reactivity of Phenyl Radicals with the Help of Distonic Charges: It is All About Electrostatic Catalysis".
Chem. Sci. **12**, 4800-4809 (2021) **Edge Article**
<https://doi.org/10.1039/d0sc07111k>
- (561) W. Peng, X. Qu, S. Shaik, B. Wang
"Deciphering the Enigmatic Oxygen Activation and Methane Oxidation Mechanisms by Patriculate Methane Monooxygenase"
Nature Catal. **4**, 266-273 (2021)
<https://doi.org/10.1038/s41929-021-00591-4>
- (562) C.J. Laconsay, D. Mallick, S. Shaik
"External Electric Fields Interrupt the Concerted Cope Rearrangement of Semibullvalene"
J. Org. Chem. **86**, 731-738 (2021)
<https://doi.org/10.1021/acs.joc.0c02322>
- (563) S. Radenković, S. Shaik, B. Braida
"Na...B Bond in NaBH₃: Solving the Conundrum"
Angew. Chem. Int. Ed. **60**, 12723-12726 (2021). <https://doi.org/10.1002/anie.202100616>
- (564) S. Shaik
"Stories of My Journey Through Valence Bond Theory, DFT, MD and their Applications to Complex Objects."
Isr. J. Chem. **62**,. e202000090 (1 of 34) (2022)
<https://doi.org/10.1002/ijch.202000090>
- (565) P.C. Hiberty, D. Danovich, S. Shaik
"A Conversation on New Types of Chemical Bonds"

- Isr. J. Chem.* **61**, (2021)
<https://doi.org/10.1002/ijch.202000114>
- (566) Y. Kapon, A. Saha, T. Duaniyas-Assaf, T. Stuyver, A. Ziv, T. Metzger, S. Yochelis, S. Shaik, R. Naaman, M. Reches, Y. Paltiel
 “Evidence for New Enantiospecific Interaction Force in Chiral Biomolecules”
Chem., **7**, 2787-2799 (2021).
<https://doi.org/10.1016/j.chempr.2021.08.002>
- (567) Z. Wang, S. Shaik, B. Wang
 “Conformational Motion of Ferredoxin Enables Efficient Electron Transfer to heme in the Full-Length P450_{TR}”
J. Am. Chem. Soc. **143**, 1005-1016 (2021)
<https://dx.doi.org/10.1021/jacs.0c11279>
- (568) T. Stuyver, S. Shaik
 “Detecting and Conceptualizing Reaction Modes through Promotion Energy Analysis: Nucleophilic and Electrophilic Aromatic Substitution Reactions”
J. Am. Chem. Soc. **143**, 4367-4378 (2021)
<https://dx.doi.org/10.1021/jacs.1c00307>
- (569) S. Shaik, D. Danovich, P.C. Hiberty
 “Valence Bond Theory – Its Birth, Struggles with Molecular Orbital Theory, Its Present State and Future Prospects”
Molecules, **26**, 1624 (2021)
<https://doi.org/10.3390/molecules26061624>
- (570) CHAPTER
 T. Stuyver, S. Shaik
 “Bridging Conceptual Density Functional and Valence Bond Theories”
 Chapter 20 In: *Conceptual Density Functional Theory. Towards New Chemical Reactivity Theory*. S. Liu, Editor. Wiley VCH, 2022.
<https://doi.org/10.1002/9783527829941.ch20>
- (571) J. Joy, D. Danovich, S. Shaik
 “The Nature of the Trigger Bond in Explosive Materials”.
J. Org. Chem. **86**, 15588-15596 (2021)
<https://doi.org/10.1021/acs.joc.1c02066>
- (572) T. Stuyver, S. Shaik
 “Resolving Entangled Reactivity Modes Through External Electric Fields and Substitution: Application to E2/S_N2 Reactions”.
J. Org. Chem. **86**, 9030-9039 (2021)
<https://doi.org/10.1021/acs.joc.1c01010>
- (573) T. Stuyver, Frank De Proft, Paul Geerling, S. Shaik
 “Correction to: ‘How Do Local Reactivity Descriptors Shape the Potential Energy Surface Associated with Chemical Reactions? The Valence Bond Delocalization Perspective’
J. Am. Chem. Soc. **143**, 10102-10113 (2021)
<https://doi.org/10.1021/jacs.0c02390>
- (574) X. Zhang , Y. Jiang, Q. Chen, S. Dong, Y. Feng. Z. Cong, S. Shaik, B. Wang
 “H-Bonding Networks Dictate the Molecular Mechanism of H₂O₂ Activation by P450”
Acs. Catal. **11**, 8774-8785 (2021).
<https://doi.org/10.1021/acscatal.1c02068>
- (575) J. Feng, S. Shaik, B. Wang,
 “Spin-regulated electron transfer and exchange-enhanced reactivity in Fe₄S₄-mediated redox reaction of the Dph2 Enzyme During the Biosynthesis of Diphthamide”
Angew. Chem. Int. Ed. **60**, 20430-20436 (2021)
<https://doi.org/10.1002/anie.202107008>
- (576) S. Shaik, K. D. Dubey
 “The Catalytic Cycle of Cytochrome P450 – A Fascinating Choreography”
Trends in Chemistry, **3**, 1027- 1044 (2021)
<https://doi.org/10.1016/j.trechm.2021.09.004>
- (577) V. Pomogawv, S. Lee, S. Shaik, M. Filatov, C.H. Choi
 “Exploring Dyson’s Orbitals and Their Electronic Binding Energies for Conceptualizing Excited States from Response Methodology”
J. Phys. Chem. Lett., **12**, 9963-9972 (2021)

- (578) <https://doi.org/10.1021/acs.jpcelett.1c02494>
Y. Mo, D. Danovich, S. Shaik
“The Roles of Charge Transfer and Polarization in Non-Covalent Interactions: A Perspective from Ab Initio Valence Bond Methods”.
J. Mol. Modelling, **28** (2022)
<https://doi.org/10.1007/s00894-022-05187-8>
- (579) EDITING
S. Shaik, T. Stuyver, Editors
“Electric Fields and Structure-Reactivity Aspects: New Horizons in Chemistry”
The Royal Society of Chemistry, 2021, pp. 1-421
<https://doi.org/10.1039/9781839163043>
- (580) J.M. Galbraith, S. Shaik, D. Danovich, B. Braida, W. Wu, P.C. Hiberty, D.L. Cooper, P.B. Karadakov, T. H. Dunning
“Valence Bond and Molecular Orbital: Two Powerful Theories that Nicely Complement One Another”
J. Chem. Ed. **98**, 3617-3620 (2021)
<https://doi.org/10.1021/acs.jchemed.1c00919>
- (581) S. Kalita, S. Shaik, K. D. Dubey
“MD Simulations and QM/MM Calculations Reveal the Key Mechanistic Elements which are Responsible for Efficient C-H Amination Reaction Performed by a Bioengineered P450 Enzyme”
Chem. Sci. **12**, 14507-14518 (2021)
<https://doi.org/10.1039/D1SC03489H>

2022

- (582) S. Dorđević, S. Radenković, S. Shaik, B. Braida
“On the Nature of the Bonding in Coinage-Metal Halides”
Molecules, **27**, 490 (2022).
<https://doi.org/10.3390/molecules27020490>
- (583) O. Eisenstein, S. Shaik
PREFACE: “Computational Catalysis: A Land of Opportunities”
Topics in Catalysis, **65**, 1-6 (2022).
<https://doi.org/10.1007/s11244-021-01555-5>
- (584) S. Yadav, S. Shaik, S. Kalita, K. D Dubey
“Local Electric Fields Dictate Function: The Different Product Selectivity for Fatty Acid Oxidation by Two Deceptively Very Similar P450 Peroxygenases OleT and BS_β”.
J. Chem. Information and Modelling. **62**, 1025-1035 (2022)
<https://doi.org/10.1021/acs.jcim.1c01453>
- (585) S. Wang, P. Ma, S. Shaik, H. Chen
“Valence-Inversed States of Nickel(II) Complexes Perform Facile C-H Bond Activation”
J. Am. Chem. Soc. **144**, 14607-14613(2022)
<https://doi.org/10.1021/jacs.2c03835s>
- (586) EDITING
O. Eisenstein, S. Shaik, Editors
“Computational Catalysis: A Land of Opportunities”
TOPICS in CATALYSIS, **65**, 1-6 (2022).
Issues 1-4: pp 6-562.
Springer, Germany, 2022.
- (587) S. Kalita, S. Shaik, K.D. Dubey
“Mechanistic Conundrum of C-C Bond Cleavage by CYP51”
ACS Catal. **12**, 5673-5683 (2022)
<https://pubs.acs.org/doi/10.1021/acscatal.2c00111>.
- (588) S. Yadav, S. Shaik, S. Kalita, K.D. Dubey
“Local Electric Fields Dictate Function: The Different Product Selectivity for Fatty Acid Oxidation by Two Deceptively Very Similar P450 Peroxygenases OleT and BS_β”.
J. Chem. Information and Modelling. **62**, 1025-1035 (2022)
<https://doi.org/10.1021/acs.jcim.1c01453>
- (589) B. Wang, P. Wu, S. Shaik
“Critical Roles of Exchange and Super-Exchange Interactions in Dictating Electron Transfer and Reactivity in Metalloenzymes?”

- J. Phys. Chem. Lett.* 2022, **13**, 2871–2877
<https://doi.org/10.1021/acs.jpcllett.2c00513>
- (590) B. Wang, X. Zhang, W. Fang, C. Rovira, S. Shaik
 “How Do Metalloproteins Tame the Fenton Reaction and Utilize HO• Radicals in Constructive Manners?”
Acc. Chem. Res., **55**, 2280-2290 (2022)
<https://doi.org/10.1021/acs.accounts.2c00304>
- (591) P. Wu, Y. Gu, L. Liao, J. Jin, Z. Wang, J. Zhou, S. Shaik, B. Wang
 “Coordination Switch Derives the Selective C-S Bond Formation by the Nonheme Sulfoxide Synthases”
Angew. Chem. Int. Ed., e202214235 (1 of 9) (2022)
<https://doi.org/10.1002/anie.202214235>
- (592/910) S. Shaik, D. Danovich, P.C. Hiberty
 “On the Nature of the Chemical Bond in Valence Bond Theory”
J. Chem. Phys. **157**, 090901 (2022) (pp. 1-44) <https://doi.org/10.1063/5.0095953>
- (593) Y. Mo, D. Danovich, S. Shaik
 “On the Nature of the Chemical Bond According to Valence Bond Theory”
 “The Roles of Charge Transfer and Polarization in Non-Covalent Interactions: A Perspective from Ab Initio Valence Bond Methods”.
J. Mol. Modelling, **28**, 274, pp. 1-16 (2022)
<https://doi.org/10.1007/s00894-022-05187-8>
- (594) W. Peng, S. Yan, X. Zhang, L. Liao, J. Zhang, S. Shaik, B. Wang
 “How do preorganized electric fields function in catalytic cycles? The Case of the enzyme tyrosine hydroxylase”
J. Am. Chem. Soc. **144**, 20484-20494 (2022)
<https://doi.org/10.1021/jacs.2c09263>
Noted by the Editor in Chief. E. Carriera
- (595) P.G. Kusalik, M.E. Gracheva, S. Shaik, N. J. English
 “New Perspectives on Molecular Simulation of Chemistry and Physics in External Fields”.
Phys. Chem. Chem. Phys. e28660 (2022) pages 1-2. Editorial
<https://doi.org/10.1039/D2CP90209E>
- (596 =564) S. Shaik
 “Stories of My Journey Through Valence Bond Theory, DFT, MD and their Applications to Complex Objects”.
Isr. J. Chem. **62**, 1-34 (2022); e202000090.
<https://doi.org/10.1002/ijch.202000090>

2023-2024

- (597) EDITING
 S. Shaik, P.C. Hiberty, Editors
 “Introduction to the Valence Bond Section of the MRW Project”.
 Part of the Multi Reference Works (MRW).
 In “Comprehensive Computational Chemistry”.
 Elsevier, Netherlands, 2024.
1, 252-254 (2024).
[doi:10.1016/B978-0-12-821978-2.00063-5](https://doi.org/10.1016/B978-0-12-821978-2.00063-5)
- (598) CHAPTER
 P.C. Hiberty, S. shaik
 “Understanding VB Theory”
 Part of the Multi Reference Works (MRW). Elsevier, Netherlands, 2024
1, 255-275 (2024).
[doi:10.1016/B978-0-12-821978-2.00014-3](https://doi.org/10.1016/B978-0-12-821978-2.00014-3)
- (599) CHAPTER
 P.C. Hiberty, S. Shaik
 “The Breathing-Orbitals Valence Bond Method: A VB Method That Includes Dynamic Electron Correlation. The Section on Valence Bond Theory. Part of the Multi Reference Works (MRW). Elsevier, Netherlands, 2024
 Chapter 3 in “Comprehensive Computational Chemistry: The Valence Bond Section”.
1, 311-330 (2024).
[doi:10.1016/B978-0-12-821978-2.00001-5](https://doi.org/10.1016/B978-0-12-821978-2.00001-5)
- (600) CHAPTER
 S. Shaik, D. Danovich, J. Joy, P.C. Hiberty
 “Valence Bond Diagrams and Chemical Reactivity”

- Section on Valence Bond Theory. Part of the Multi Reference Works (MRW).
In "Comprehensive Computational Chemistry". Elsevier, Netherlands, 2024
684-711 (2024).
[doi:10.1016/B978-0-12-821978-2.00002-7](https://doi.org/10.1016/B978-0-12-821978-2.00002-7)
- (601) X. Zhang, Z. Wang, Z. Li, S. Shaik, B. Wang
"[4Fe-4S]-Mediated Proton-Coupled Electron Transfer Enables the Efficient Degradation of Chloro-alkenes by Reductive Dehalogenases"
ACS Catal. **13**, 1173-1185 (2023)
<https://doi.org/10.1021/acscatal.2c06306>
- (602) Y. Wu, C. Zhao, Y. Su, S. Shaik, W. Lai
"Mechanistic Insights into Peptidyl-Cysteine Oxidation by Copper-Dependent Formylglycine-Generating Enzyme".
Angew. Chem. Int. Ed. e20212053 (1-6) (2023)
<https://doi.org/10.1002/anie.202212053>
- (603) S. Yadav, S. Shaik, K.D. Dubey
"The Decarboxylation and Protonation Enigma in the H85Q Mutant of Cytochrome P450 OleT"
J. Phys. Chem. B. **127**, 2927-2933 (2023)
<https://doi.org/10.1021/acs.jpcc.3c00143>
- (604) S. Jain, D. Danovich, S. Radenkovich, S. Shaik
"Dichotomy of Delocalization/Localization and Charge-Shift Bonding in Germanazene and Its Heavier Group 14 Analogues: A Valence Bond Study"
Chem. Eur. J. e202300992 (1 of 9) (2023)
<https://doi.org/10.1002/chem.202300992>
- (605) S. Kalita, H. Bergman, K.D. Dubey, S. Shaik
"How Can Static and Oscillating Electric Fields Serve in Decomposing Alzheimer's Plaques?"
J. Am. Chem. Soc. **145**, 3543-3553 (2023)
<https://doi.org/10.1021/jacs.2c12305>
*** Noted by the Editor in Chief. E. Carriera**
- (606) Z. Wang, W. Diao, P. Wu, Y. Fu, Z. Cao, S. Shaik, B. Wang
"How the Conformational Movement of the Substrate Drives the Regioselective C-N Bond Formation in P450 TleB: Insights from Molecular Dynamics Simulations and Quantum Mechanical/Molecular Mechanical Calculations".
J. Am. Chem. Soc. **145**, 7252-7267 (2023).
<https://doi.org/10.1021/jacs.2c12962>
Noted by the Editor in Chief. E. Carriera
- (607) S. Shaik, K. D. Dubey,
"Nanomachines in Living Matters: The Soft-Robot Cytochrome P450"
Trends in Chemistry, **5**, 763-744 (2023).
<https://doi.org/10.1016/j.trechm.2023.07.002>
Highlighted in five international sites/magazines*
- (608) K. Gorankumar, S. Shaik, R. Ramanan
"Two-Ways Catalysis in Diels-Alder Reaction Limits the Extent of Inhibition Induced by External Electric Field Stimuli: Implications on Reaction Mechanism and Stereoselectivity"
Angew. Chem. Int. Ed. **2023**, e202307579
<https://doi.org/10.1002/anie.202307579>
- (609) N. Kuriakose, S. Shaik
"Oriented External Electric Field Effects on the Activation of Aryl C-O Bond in Anisole Using Rh(PEP) (E=Al, B, Ga) Catalysts".
Chem. Eur. J. **2023**, e202300977 (1 of 9). <https://doi.org/10.1002/chem.202300977>
*** A HOT PAPER**
- (610) C. Tang, T. Stuyver, Y. Ye, J.-Y. Liu, J. Shi, S. Shaik, H. Xia, W. Hong
"Voltage-Driven Control of Single-Molecule Keto-Enol Equilibrium in a Two-Terminal Junction System"
Nature Commun., **14**, 3657 (2023). <https://doi.org/10.1038/s41467-023-39198-7>
*** Featured by the editors of Nature Communications among the Editors' Highlights webpage:**
<https://www.nature.com/ncomms/>
- (611) L.H. Javitt, S. Kalita, K.D. Dubey, D. Ehre, S. Shaik, M. Lahav, I. Lubomirsky
"Electro-freezing of Supercooled Water Is Induced by Hydrated Al³⁺ and Mg²⁺ Ions: Experimental and Theoretical Studies".
J. Am. Chem. Soc. **145**, 18904-18911 (2023).

- <https://doi.org/10.1021/jacs.3c05004>
 (612) G. Cassone, Saija, S. Franz, S. Shaik
 “The Reactivity-Enhancing Role of Water in Ammonia-Aqueous Solution”
J. Phys. Chem. Lett., **14**, 7808-7813 (2023).
<https://doi.org/10.1021/acs.jpcllett.3c01810>
- (613) S.A. Siddiqui, S. Shaik, S. Kalita, K.D. Dubey
 “A Porphyrin-Based Molecular Cage Guided by Designed Local-Electric Field Is Highly Selective and Efficient”
Chem. Sci. **14**, 10329-10339 (2023), Advanced Article.
<https://doi.org/10.1039/d3sc01720f>
- (614) S. Shaik, D. Danovich, R.N. Zare
 “Valence Bond Theory Allows a Generalized Description of Hydrogen Bonding”
J. Am. Chem. Soc. **145**, 20132-20140 (2023).
<https://doi.org/10.1021/jacs.3c08196>
- (615) **EDITING**
 Y. Apeloig, S. Shaik
 “New Frontiers in Gas Phase Chemistry and Catalysis. Celebrating the 800th Birthday of Helmut Schwarz.
 Foreword: *Isr. J. Chem.* 2023, 63, e202300106 (1 of 4)
doi.org/10.1002/ijch.202300106.
- (616) S.A. Siddiqui, T. Stuyver, S. Shaik and K.D. Dubey
 “Designed Local Electric Fields –Promising Tools for Enzyme Engineering”
J. Am. Chem. Soc. Au, **3**, (12) 3259-3269 (2023).
<https://doi.org/10.1021/jacsau.3c00536>

2024

- (617) S. Yadav, S. Shaik, K.D. Dubey
 “On the Engineering of Reductase-Based-Monooxygenase Activity in CYP450 Peroxygenases”
Chem. Science, **15**, 5174-5186 (2024)
<https://doi.org/10.1039/D3SC06538C>
- (618) Q. Zhang, Q. Chen, S. Shaik, B. Wang
 “Flavin-N5OOH Functions as Both a Powerful Nucleophile and Base in the Supperfamily of Flavoenzymes”
Angew Chem. Int. Ed. (2024) e202318629
<https://doi.org/10.1002/anie.202318629>
- (619) S. Shaik
 “My Vision of the Future of Electric-Field-Aided Chemistry in 2050”.
ACS Phys. Chem. Au, **4** (3) 191-201 (2024).
<https://doi.org/10.1021/acspchemau.3c00064>
*** Featured on February 14, 2024 by the editors of Chemistry World in the MUST READ Selection:
 Sason Shaik’s vision of electric-field-aided chemistry in 2050**
- (620) S. Shaik, A. S. Travis
 “Chemistry at the Hebrew University of Jerusalem, 1948-1967”.
 841-877 (2024)
 In: “THE HISTORY OF CHEMISTRY AT HEBREW UNIVERSITY OF JERUSALEM : The Nation-State and
 Higher Education”. Eds. Y. Weiss, U. Rebhun
 The Hebrew University Magnes Press, Jerusalem, 2024
 ששון צחייק, אנתוני ס” טראוויס
 “לימודי הכימיה באוניברסיטה העברית, 1967-1948”
- (621) S. Jain, D. Danovich, S. Shaik
 “Dinitrogen Activation within Frustrated Lewis Pairs is Promoted by Adding External Electric Fields”.
J. Phys. Chem. A, **128**, 4595–4604 (2024).
<https://doi.org/10.1021/acs.jpca.4c00437>
- (622/968) D. Danovich, A. Tkachenko, S. Alvarez, S. Shaik
 “A Gravitational-Like Relationship of Dispersion Interactions is Exhibited by 40 Pairs of Molecules and Noble
 Gas Atoms”.
J. Am. Chem. Soc. **146**, 31198-31024 (2024).
<https://doi.org/10.1021/jacs.4c11211>
*** Noted the by Editor In Chief, Carriera.**
- (623) S. Siddiqui, S. Shaik, K.D. Dubey

“A Designed CYP450 Scaffold that Possesses a Local Electric Field Biodegrades Polyethylene Terephthalate (PET)”.

ACS Catal. **14**, 15108-15122 (2024)

<https://doi.org/10.1021/acscatal.4c05363>

2025

- (624) S. Jain, D. Danovich, S. Radenković, S. Shaik,
“Unraveling the Bonding, Structure, and Aromaticity of Pentazole, Pentaphosphole, and Cyclopentadiene Anions: A Comprehensive Study”.
J. Am. Chem. Soc. **147**, 1092-1100 (2025)
<https://doi.org/10.1021/jacs.4c14515>
- (625) S. Kalita, D. Danovich and S. Shaik,
“Origins of the Superiority of Oscillating Electric Fields for Disrupting Senile Plaques: Insights from the 7-Residue and Full-Length A β -42 Peptide”.
J. Am. Chem. Soc. **147**, 2626-2641 (2025).
<https://doi.org/10.1021/jacs.4c14791>
- (626/977) Z. Xuan, L.-T. Wang, B. Wang, L. Jia, S. Shaik, J. Zhou, B. Wang
“An Alternative Mechanism for C–C Desaturation Underscores a Dual-Controlled Mechanism for the Fate of Radical Intermediate in Iron(II)- and 2-(Oxo)glutarate-Dependent Oxygenase DfmD”
J. Am. Chem. Soc., XXX. XXX -XXX (2025).
<https://doi.org/10.1021/jacs.5c02361>
- (627/955) BOOK
S. Shaik, D. Danovich, P.C. Hiberty
“A Chemist Guide to Valence Bond Theory”
2nd Edition, Wiley 2025
In Press
- (628/970) D. Samanta, S. Sakar, D. Singh, S. Samanta, S. Manna, K.D. Dubey, A Dey, S. Shaik, S.P. Rath
“Unusually Stable Synthetic Diheme *bis*-Fe(IV)oxo: An Intermediate in Diheme Enzymes *MauG* and *BthA*”
J. Am. Chem. Soc. In Press. DOI: 10.1021/jacs.5c03000
- (629/993) D. Singh, E.S.S. Kumar, S. Shaik*, and K.D. Dubey*
“The Manner Whereby Enzymes Designed by Machine Learning Exploit Pre-Organized Electric Fields for Efficient Carbene Transfer”.
Nature Communications., submitted
- (630/994) Y. Wang, S. Shaik, B. Wang
“Cytochrome P450 that is Controlled by the Proton Channel of the Protein”.
ACS Catal., In press. Xxx.xxx.xxx.

Notes on Publications:

***[493] Highlighted This book is among the best-selling Chemistry eBooks at all times:**

<https://bookauthority.org/books/best-selling-chemistry-ebooks>

An example of a Top Review for the book can be found in Amazon. See e.g. the following:

Top reviews from other countries



bookworm8

5.0 out of 5 stars

Unusual, intriguing read for laypeople as well as chemistry teachers and students.
Reviewed in the United Kingdom on July 26, 2016.

Written as a guide to a new way of teaching chemistry, aimed at teachers, this is an interesting read. My grasp of chemistry is not great these days, as I have not studied it since leaving school in 1961 so I not only enjoyed this book but learnt a lot too! Luckily one of my sons studied chemistry at A-level and helped me at times and I would recommend that any non-specialist readers have similar backup. As a retired teacher myself, the approach was very engaging and the layout logical and helpful. The illustrations and images are invaluable, the vocabulary manageable and the pace - although a bit fast for me at times- was good overall. Drawing together techniques from many areas to make the teaching of chemistry (at degree level, in this book) very relevant and engaging, I think this book is a success on many levels. The 'conversations' between Shaik and his collaborators add both intro and conclusion to the lectures, and are so helpful in enabling readers to understand the aims of the lectures, the construction analogy is accessible, the love of chemistry and of chemistry-teaching shines through every chapter, and the referencing throughout is impeccable. I loved the chapter on the Lego principle, featuring the periodic table, of course. I have a friend who, as a scientist and a superb embroiderer, made an amazing exhibition piece based on the periodic table. Since reading this book, the selection she made of which elements to give extra attention to piece even more interesting - I would love the author to see this piece of work, he would, I feel sure, enjoy it as much as the audience of Embroiderers did when it was exhibited! A superb read, not just for chemistry students and teachers.

***[590] Highlighted**

Dear Colleague,
Congratulations!

I am pleased to let you know that several of your articles published between 2020-2021 are some of our most highmost cited publications, including *Electric-Field Mediated Chemistry: Uncovering and Exploiting the Potential of (Oriented) Electric Fields to Exert Chemical Catalysis and Reaction Control* ([10.1021/jacs.0c05128](https://doi.org/10.1021/jacs.0c05128)).

Thank you for publishing with *JACS* –

I look forward to receiving more of your first-class science in the future.

Sincerely,

Erick M. Carreira
Editor-in-Chief
Journal of the American Chemical Society

*** [605] Noted by Editor in Chief Carreira**

*** [607] Highlighted**

Discovery in nanomachines within living organisms -- cytochromes P450 (CYP450s) unleashed as living soft robots (Science Daily)

<https://www.sciencedaily.com/releases/2023/08/230807121907.htm>

Discovering nanomachines within living organisms: Cytochromes P450 unleashed as living soft robots (Phys.Org. News)

<https://phys.org/news/2023-08-nanomachines-cytochromes-p450-unleashed-soft.html>

ScienceDaily: Cytochromes P450 (CYP450s) Unleashed as Living Soft Robots: Nanomachine Discovery within Living Organisms

<https://www.bollyinside.com/news/latest-science-news/sciencedaily-cytochromes-p450-cyp450s-unleashed-as-living-soft-robots-nanomachine-discovery-within-living-organisms/>

Discovery in nanomachines within living organisms — cytochromes P450 (CYP450s) unleashed as living soft robots (Crumpe)

<https://www.crumpe.com/2023/08/discovery-in-nanomachines-within-living-organisms-cytochromes-p450-cyp450s-unleashed-as-living-soft-robots/>

Living Organisms Unleash Nanomachines: CYP450s Revealed (Mirage News)

<https://www.miragenews.com/living-organisms-unleash-nanomachines-cyp450s-1061187/>

Key Enzyme for Drug Metabolism Exhibits Soft Robotic Properties Which Could Lead to Advanced Biogels and Polymers, According to Hebrew University Researchers
<https://www.pharmiweb.com/press-release/2023-08-15/key-enzyme-for-drug-metabolism-exhibits-soft-robotic-properties-which-could-lead-to-advanced-biogels-and-polymers-according-to-hebrew-university-researchers>

* [609] A HOT PAPER

* [610] Featured by the editors of Nature Communications among the Editors'

Highlights webpage: <https://www.nature.com/ncomms/>

*[619] Highlighted as a MUST-READ paper, in the "must read" section of "Chemistry World", February 14, 2024

Re: action - 14 Feb 2024

* [622/968] Highlighted by the editor in Chief.

Congratulations Sason Shaik on publication of ja-2024-11211n.R

Journal of the American Chemical Society 9:56 AM (29 minutes ago)

to david.danovich, david.danovich, alexandre.tkatchenko, atkatchenko, santiago.alvarez, sason, Sason.Shaik, francisco-office

02-Feb-2025

Journal of the American Chemical Society

Manuscript ID: ja-2024-11211n.R2

Manuscript Title: A Gravitational-Like Relationship of Dispersion Interactions is Exhibited by 40 Pairs of Molecules and Noble Gas Atoms

Author(s): Danovich, David; Tkatchenko, Alexandre; Alvarez, Santiago; Shaik, Sason

Dear Colleagues,

Congratulations on your publication above in JACS. I thoroughly enjoyed reading about dispersion interactions--a topic I have heard much about from my colleague Prof. Peter Chen. I look forward to receiving first-class science from you in JACS in the future.

Sincerely,

Erick M. Carreira

Editor-in-Chief

Journal of the American Chemical Society

ETH Zürich Hönggerberg HCI H335

Zürich, Switzerland

Email: jacs@jacs.acs.org