Publications of Sason Shaik

• M. Albeck, S. Shaik
"Reactions of Tellurium(IV) Halides with Anthracene and other Organic Compounds"
J. Chem. Soc. Perkin I, 1223−1229 (1975).
• M. Albeck, S. Shaik
"Identification of Tellurium Containing Compounds by Means of Mass Spectrometry"
J. Organomet. Chem., **91**, 307−313 (1975).
• N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces"
Progr. Theor. Org. Chem., **2**, 348−369 (1977).
• N.D. Epiotis, S. Shaik, J.R. Larson, F. Bernardi
"The Manifestations of Non-Bonded Attractions in the Physical Properties of Cis and Trans Olefins"
Tetrahedron, **33**, 3269−3274 (1977).
• N.D. Epiotis, J.R. Larson, R.L. Yates, W. Cherry, S. Shaik, F. Bernardi
"Theory of Structural Isomersion. Vicinal vs. Geminal Homodisubstituted Molecules"
J. Am. Chem. Soc., **99**, 7460−7464 (1977).
• 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).
• N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces. 5. Sigmatropic Shifts"
J. Am. Chem. Soc., **99**, 4936−4946 (1977).
• F. Bernardi, N.D. Epiotis, S. Shaik, K. Mislow
"Thiacylobutadiene and Thiabenzene. A Comparative Theoretical Analysis"
Tetrahedron, **33**, 3061−3067 (1977).
• BOOK
N.D. Epiotis, W. Cherry, S. Shaik, R.L. Yates, F. Bernardi
"*Structural Theory of Organic Chemistry*"
Top. Curr. Chem. (1977).
• M. Albeck, S. Shaik
"Electrochemical Decomposition of Biformylperoxide. A Quantum Mechanical Calculation"
J. Chem. Soc., Faraday Trans., **74**, 1496−1499 (1978).
• N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces. 1. Theory"
J. Am. Chem. Soc., **100**, 1−8 (1978).
• N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces. 2. Cycloadditions"
J. Am. Chem. Soc., **100**, 9−17 (1978).
• 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).
• N.D. Epiotis, S. Shaik
"Qualitative Potential Energy Surfaces. 4. Aromatic Substitution"
J. Am. Chem. Soc., **100**, 29−33 (1978).
• F. Bernardi, W. Cherry, S. Shaik, N.D. Epiotis
"The Structure of Fluoromethyl Radicals. Conjugative and Inductive Effects"
J. Am. Chem. Soc., **100**, 1352−1356 (1978).
• 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.
• S.S. Shaik
"Spin Inversion and Orbital Symmetry Conspiracy in Type A Lumiketone Rearrangement"
J. Am. Chem. Soc., **101**, 2736−2738 (1979).
• S.S. Shaik
"Triplet (2 + 2) Cycloadditions Spin Inversion Control of Stereoselectivity"
J. Am. Chem. Soc., **101**, 3184−3196 (1979).
• S.S. Shaik, N.D. Epiotis
"Spin Inversion in Triplet Diels-Alder Reactions"
J. Am. Chem. Soc., **102**, 122−131 (1980).
• 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).
• S. Shaik, R. Hoffmann, C.R. Fisel, R. Summerville
"Bridged and Unbridged M_2L_{10} Complexes"
J. Am. Chem. Soc., **102**, 4555−4572 (1980).
• 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).
• 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).
• BOOK
N.D. Epiotis, S. Shaik, W. Zander
"*Rearrangements: A Theoretical Approach" in: "Rearrangements in Ground and Excited States*"
P. De Mayo, Ed.
Academic Press, New York, 1980, pp 1−94.
• J.R. Larson, N.D. Epiotis, S.S. Shaik
"A Simple Theoretical Approach to Bond Energies"
Tetrahedron, **37**, 1205−1211 (1981).
• S.S. Shaik
"What Happens to Molecules as They React? A Valence Bond Approach to Reactivity"
J. Am. Chem. Soc., **103**, 3692−3701 (1981).
• A. Pross, S.S. Shaik
"Reactivity-Selectivity Relationships. A Quantum Mechanical Approach to Transition State Structure. Application to the S_N2 Reaction to Benzyl Derivatives"
J. Am. Chem. Soc., **103**, 3702−3709 (1981).
• S.S. Shaik, A. Pross
"S_N2 Reactivity of CH_3X Derivatives. A Valence Bond Approach"
J. Am. Chem. Soc., **104**, 2708−2719 (1982).
• 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).

10.1021/jp806628j CCC: $40.75
Published on Web 12/11/2008

• S.S. Shaik
"On the Origins of the Barrier in the S_N2 Identity Exchange"
Nouv. J. Chim., **6**, 159−161 (1982).
• A. Pross, S.S. Shaik
"Is Charge Development a Measure of S_N2 Transition State Structure?"
Tetrahedron Lett., **23**, 5467−5470 (1982).
• A. Pross, S. Shaik
"Why Do Rate-Equilibrium Relationships Break Down?"
J. Am. Chem. Soc., **104**, 1129−1130 (1982).
• 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).
• S.S. Shaik, A. Pross
"On the Origins of Reaction Barriers. Application to S_N2"
Bull. Soc. Chim. Belg., **91**, 355 (1982).
• S. Shaik
"Nobel Prize in Chemistry 1981. In the Frontier of Chemical Reactions" (in Hebrew)
Mada (Science), **26**, 130−132 (1982).
• S.S. Shaik, R. Bar
"The Problem of Metal–Metal (MM) Bond Alternation in $[MX_2(\mu\text{-}X)_{4/2}]_\infty$ Chain Polymers"
Inorg. Chem., **22**, 735−743 (1983).
• 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).
• 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).
• S.S. Shaik
"Reactivity and Reactivity-Selectivity Crossovers in S_N2"
Nouv. J. Chim., **7**, 201−203 (1983).
• 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).
• A. Pross, S.S. Shaik
"A Qualitative Valence Bond Approach to Organic Reactivity"
Acc. Chem. Res.,**16**, 363−370 (1983).
• 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).
• Y. Apeloig, S. Shaik, Eds.
"Application of Theory to Organic and Organometallic Molecules"
Isr. J. Chem., **23**, 1−152 (1983).
• 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).
• S.S. Shaik, R. Bar
"How Important is Resonance in Organic Species?"
Nouv. J. Chim., **8**, 411−420 (1984).
• S.S. Shaik, P.C. Hiberty
"When Does Electronic Delocalization Become an Important Driving Force of Molecular Shape and Stability? I. The Aromatic Sextet"
J. Am. Chem. Soc., **107**, 3089−3095 (1985)
• 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**, 1642−1649 (1985).
• 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).
• 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).
• E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik
"A New Electron Donor: Synthesis of 2,3,6,7 Tetra(ethyltellura)tetrathiafulvalene"
Tetrahedron Lett., **26**, 2783−2786 (1985).
• E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S.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).
• S.S. Shaik
"Identity S_N2 Reactions. The Relationship Between TS Geometry, Selectivity and the Mechanism of Solvent Action"
Isr. J. Chem., **26**, 367−374 (1985).
• S.S. Shaik
"The Collage of S_N2 Reactivity Patterns. A State Correlation Diagram Model"
Prog. Phys. Org. Chem., **15**, 197−337 (1985).
• D. Cohen, R. Bar, S.S. Shaik
"Nucleophilic Vinylic Substitution. A Theoretical Study"
J. Am. Chem. Soc., **108**, 231−240 (1986).
• S.S. Shaik
"Intrinsic Selectivity and its Geometric Significance in S_N2 Reactions"
Can. J. Chem., **64**, 96−99 (1986).
• S.S. Shaik, M.-H. Whangbo
"Electronic and Intramolecular Structural Localization in Conducting Organic Salts"
Inorg. Chem., **25**, 1201−1209 (1986).
• P.C. Hiberty, S.S. Shaik, G. Ohanessian, J.M. Lefour
"The π-Distortive Propensities in Benzene and Allyl Radical. A Reply to a Criticism"
J. Org. Chem., **51**, 3908−3909 (1986).
• E. Aharon-Shalom, J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik
"The 1:1 Mixed Stack Complex of Tetrathiafulvalene and 2,5-Dibenzyltetracyanoquino- dimethane (TTF:DBTCNQ) at 115K"
Isr. J. Chem., **27**, 375−380 (1986).
• S.S. Shaik, P.C. Hiberty, J.M. Lefour, G. Ohanessian
"Is Delocalization a Driving Force in Chemistry? Allyl Radical, Benzene, Cyclobutadiene and Their Isoelectronic Species"
J. Am. Chem. Soc., **109**, 363−374 (1987).
• S.S. Shaik
"Nucleophilicity and Vertical Ionization Potentials in Cation-Anion Recombinations"
J. Org. Chem., **52**, 1563−1568 (1987).
• E. Canadell, S.S. Shaik

"Potentially Conducting Organometallic Systems: the Stibaphenalenyl Series"

Inorg. Chem., **26**, 3797−3802 (1987).

• S.S. Shaik

"How is Transition State Looseness Related to the Reaction Barrier"

J. Am. Chem. Soc., **110**, 1127−1131 (1988).

• E. Buncel, S.S. Shaik, I.-H. Um, S. Wolfe

"A Theoretical Treatment of Nucleophilic Reactivity in Additions to Carbonyl Compounds. The Role of the Vertical Ionization Energy"

J. Am. Chem. Soc., **110**, 1275−1279 (1988).

• J.Y. Becker, J. Bernstein, S. Bittner, N. Levi, S.S. Shaik, N. Zer-Zion

"Synthesis and Property of Archetypical Donor-Acceptor-Donor (D2A) Molecules"

J. Org. Chem., **53**, 1689−1694 (1988).

• J. Bernstein, S.S. Shaik

"The Particle - Wave Duality. Teaching via a Visual Metaphor"

J. Chem. Educ., **65**, 339−340 (1988)

• 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).

• 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).

• 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).

• J.Y. Becker, J. Bernstein, S. Bittner, S.S. Shaik

"Strategic Design of Organic Conductors. Preparation and Characterization of EDA Complexes with Fixed Stoichiometry"

Synth. Met., **27**, 197−204 (1988).

• J.Y. Becker, J. Bernstein, S. Bittner, J.A.R.P. Sarma, L. Shahal, S.S. Shaik

"The Structure of Tetra(telluraethyl)-tetrathiafulvalene- ($TTeC_2$-TTF)"

Acta Crystallogr. C, **C44**, 1770−1772 (1988)

• S.S. Shaik, H.B. Schlegel, S. Wolfe

" Transition State Geometries and the Magnitude of S_N2 Barriers: A Theoretical Study"

J. Chem. Soc., Chem. Commun., 1322−1324 (1988).

• A. Pross, S.S. Shaik

"Structure - Reactivity Coefficients. Do They Measure Transition State Structure?"

Nouv. J. Chim., **13**, 427−434 (1989).

• S.S. Shaik, A. Pross

"Nucleophilic Attack on Cation Radicals and Cations. A Theoretical Study"

J. Am. Chem. Soc., **111**, 4306−4312 (1989).

• A. Demoliens, 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).

• G. Sini, P.C. Hiberty, S.S. Shaik

"The Origins of the Different Bonding Features in SiH_5^- and CH_5^-. A Valence Bond Curve Crossing Model"

J. Chem. Soc., Chem Commun., 772−774 (1989).

• G. Sini, S.S. Shaik, J.M. Lefour, G. Ohanessian, P.C. Hiberty

"Quantitative Curve Crossing Computation of a Model S_N2 Reaction $H^- + CH_3H' \rightarrow HCH_3 + H'^-$"

J. Phys. Chem., **93**, 5661−5665 (1989).

• J.Y. Becker, J. Bernstein, S. Bittner, J.A.R.P. Sarma, S.S. Shaik

"Structural Trends in Potential Conductors Based on (D-$CH_2)_2$TCNQ Molecules"

Chem. Mater., **1**, 412−420 (1989).

• S.S. Shaik

"*A Qualitative Valence Bond Approach to 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.

• S.S. Shaik, E. Canadell

"Regioselectivity of Radical Attacks on Substituted Olefins. Application of the SCD Model"

J. Am. Chem. Soc., **112**, 1446−1452 (1990).

• P. Maitre, P.C. Hiberty, G. Ohanessian, S.S. Shaik

"Quantitative Curve Crossing Computations of Curve Crossing Diagrams for Model Atom Exchange Reactions"

J. Phys. Chem., **94**, 4089−4093 (1990).

• G. Sini, G. Ohanessian, P.C. Hiberty, S.S. Shaik

"Why is SiH_5^- a Stable Intermediate While CH_5^- is a Transition State? A Quantitative Curve Crossing Valence Bond Study"

J. Am. Chem. Soc., **112**, 1407−1413 (1990).

• S.S. Shaik

"S_N2 Reactivity and its Relation to Electron Transfer Concepts"

Acta Chem Scand., **44**, 205−221 (1990).

• L. Eberson, 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).

• P. Maitre, F. Volatron, P.C. Hiberty, S.S. Shaik

"Hypercoordination in SiH_5^- and $SiH_5\cdot$. Electron-Count Dependence"

Inorg. Chem., **29**, 3047−3048 (1990).

• 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).

• 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).

• S.S. Shaik, J.P. Dinnocenzo

"Nucleophilic Cleavage of One-Electron σ Bonds are Predicted to Proceed with Stereoinversion"

J. Org. Chem., **55**, 3434−3435 (1990).

• S.S. Shaik, P.C. Hiberty

"Curve Crossing Diagrams as General Models for Chemical Reactivity and Structure"

"*Theoretical Concepts for Chemical Bonding*", Invited Review, **4**, 324−378 (1991)

• S.S. Shaik

"The LEGO Way: Curve crossing Diagrams as General Models in Physical Organic Chemistry"

Pure Appl. Chem., **63**, 195−204 (1991).

• J.Y. Becker, J. Bernstein, S. Bittner, L. Shahal, S.S. Shaik

"Preparation of Bromotetrathiafulvalene and 1,2-Dibromotetrathiafulvalene"

J. Chem. Soc., Chem. Commun., 92−93 (1991).

• G. Sini, P. Maitre, P.C. Hiberty, S.S. Shaik

" Covalent, Ionic and Resonating Single Bonds"

J. Mol. Struct. (THEOCHEM), **229**, 163−188 (1991).

• 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**−**31**, 2523−2528 (1991).

• S.S. Shaik

"Valence Bond Mixing: The LEGO Way. From Resonating Bonds to Resonating Transition States"

An Encomium to Linus Pauling.

"*Molecules in Natural Science and Medicine*", Z.B. Maksic, M. E. Maksic, Eds.

Ellis Horwood, London, 1991.

• 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).

• S. Goldstein, G. Czapski, H, Cohen, D. Meyerstein, J.K. Cho, S. Shaik

"Deamination of 2-methyl-2-propylamine Induced by Hydroxyl Radicals and Metal Ions. A Comparison between the Rate of β Elimination of Ammonia and Water"

Inorg. Chem., **31**, 798−803 (1992).

• A. Pross, S. Shaik

"What is a Good Approximation for the Transition State of an Organic Reaction?"

Croat. Chem. Acta, **31**, 625−631 (1992).

• E. Heilbronner, S. Shaik

"Fluctuating Double-Bond Localization and Charge Migration in π-System"

Helv. Chim. Acta, **75**, 539−556 (1992).

• S. Shaik, P. Maitre, 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).

• G. Sini, S. Shaik, P.C. Hiberty

"Quantitative Valence Bond Computations of Curve Crossing Diagrams for A Gas Phase S_N2 Reactions, $F^- + CH_3F \rightarrow FCH_3 + F^-$"

J. Chem. Soc., Perkin Trans., 2, 1019−1025 (1992).

• A. Ioffe, S. Shaik

"Intramolecular Catalysis: Electronic and Entropic Effects in the Cycloaddition of Three Ethylenes vs the Diels-Alder reactions"

J. Chem Soc., Perkin Trans., 2, 2101−2108 (1992).

• 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.

• 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).

• 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).

• S. Goldstein, G. Czapski, H, Cohen, D. Meyerstein, S. Shaik

"The Effect of N-Alkylation on The Rate of β-Amino Elimination from transients with Cu^{II}–Carbon σ-Bonds"

J. Chem. Soc., Faraday Trans., **89**, 4045−4051 (1993).

• Y. Apeloig, O. Merin-Aharoni, D. Danovich, 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?"

Isr. J. Chem., **33(4)**, 387−402 (1993).

• 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).

• C. Lifshitz, Y. Gutkis, 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).

• C. Lifshitz, Y. Gutkis, J. Laskin, A. Ioffe, S. Shaik

"Threshold Formation of Benzylium (Bz^+) and Tropylium (Tr^+) From Toluene. Nonstatistical behavior in Franck-Condon Gaps"

J. Phys. Chem., **97**, 12291−12295 (1993)

• S. Shaik

"A Primer for Valence Bond Mixing and Avoided Crossing: General Paradigms in Chemical Reactivity"

J. Mol. Liq., **61**, 49−79 (1994).

• 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).

Isr. J. Chem., **33**, part B 353−457 (1993).

• S. Shaik, A. Ioffe, A.C. Reddy, A. Pross

"What is A Good Approximation for Transition State Structure? Menshutkin and Ionic S_N2 Reactions"

J. Am. Chem. Soc., **116**, 262−273 (1994).

• 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).

• 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).

• 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-Methylcholantrene 11,12-Oxide to the Corresponding β-Amino-Alcohol Derivatives"

Tetrahedron Lett., **50**, 8505−8514 (1994).

• 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**, 391−394 (1994).

• A. Valdman, S. Ruhman, S. Shaik, G.N. Sastry
" Coherent Photochemistry in Solution: Impulsive Photoselective Photolysis of $Mn_2(CO)_{10}$"
Chem. Phys. Lett., **230**, 110−116 (1994).
• 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 Cleavage of σ-Cation Radicals"
J. Am. Chem. Soc., **117**, 3205−3222 (1995).
• S. Shaik, P.C. Hiberty
"VB Mixing and Curve Crossing Diagrams in Chemical reactivity and Bonding"
Adv. Quant. Chem., **26**, 99−163 (1995)
• P.C. Hiberty, D. Danovich, A. Shurki, S. Shaik
"Why Does Benzene Possess a D_{6h} Symmetry? A Quasiclassical Approach for Probing π-Bonding and Delocalization Energy"
J. Am. Chem. Soc., **117**, 7760−7768 (1995).
• 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).
• A.C. Reddy, D. Danovich, S. Shaik
"Electron Transfer Mechanistic Manifold and Variable Transition State Character. A Theoretical Investigation of Model Electron Transfer Processes Between Nucleophiles and Cation Radicals"
J. Chem. Soc. Perkin Trans., 2, 1525−1539 (1995).
• 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).
• 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).
• G.N. Sastry, A.C. Reddy, S. Shaik
"Orbital Selection Rules and Their Structural Consequences in the Electron Transfer and Polar Reactions of Cyclizable Anion Radicals"
Angew. Chem., Int. Ed., **34**, 1495−1497 (1995).
• G.N. Sastry, A.C. Reddy, S. Shaik
"Orbital Selection Rules and Their Structural Consequences in the Electron Transfer and Polar Reactions of Cyclizable Anion Radicals"
Angew. Chem., **107**, 1619−1621 (1995).
• S. Shaik, D. Danovich, A. Fiedler, D. Schröder, H. Schwarz
"Two-State-reactivity in Organometallic Gas Phase Ion Chemistry"
Helv. Chem. Acta, **78**, 1393−1407 (1995).
• 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 $C_2H_4^+/NH_3$ Pair"
J. Chem. Soc., Perkin Trans., 2, 1717−1719 (1995).
• 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).
• 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).
• G.N. Sastry, D. Danovich and S. Shaik
"Towards the Definition of Maximum Allowable Tightness of an Electron transfer Transition State in the Reactions of Anion radicals and Alkyl Halides"
Angew. Chem., Int. Ed., **35**, 1098−1100 (1996).
• G.N. Sastry, D. Danovich, S. Shaik
"Towards the Definition of Maximum Allowable Tightness of an Electron transfer Transition State in the Reactions of Anion radicals and Alkyl Halides"
Angew. Chem., **108**, 1208−1211 (1996).
• S. Shaik, S. Zilberg, Y. Haas
"A Kekulé-Crossing Model for the Anomalous behavior of the b_{2u} Modes of Polyaromatic Hydrocarbons in the Lowest Excited $^1B_{2u}$ State"
Acc. Chem. Res., **29**, 211−218 (1996).
• 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).
• 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).
• E.M. Conwell, J. Perlstein, S. Shaik
"Interchain Photoluminescence in Poly (phenylene vinylene) Derivatives"
Phys. Rev. B, **54**, part II, R2308-R2310 (1996)
• H. Zuilhof, J.P. Dinnocenzo, A.C. Reddy, S. Shaik
"A 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).
• L. Eberson, R. González-Luque, M. Merchán, F. Radner, B.O. Roos, S. Shaik
"Radical Cations of Nonalternant Systems as Probes of the Shaik-Pross VB Configuration Mixing Model"
J. Chem. Soc., Perkin Trans., 2, 463−472 (1997).
• 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).
• S. Shaik, A. Shurki, D. Danovich, P.C. Hiberty
"A Different Story of Benzene"
The Proceeding of the WATOC Conference, July 1996
J. Mol. Struct. (THEOCHEM), **398**−**399**, 155−167 (1997).
• S. Shaik, D. Danovich, G.N. Sastry, P.Y. Ayala, H.B. Schlegel
"Dissociative Electron Transfer and Substitution Reactions of Ketyl Radical Anions and Methyl Chloride. Differences and Difficulties in their Reaction Paths"
J. Am. Chem. Soc., **119**, 9237−9245 (1997).
• J.N. Harvey, D. Schröder, W. Koch, D. Danovich, S. Shaik, H. Schwarz
"Electron Transfer Reactivity in the Bond Activation of Organic Fluorides by Calcium Monocation"
Chem. Phys. Lett., **273**, 164−170 (1997).
• J.N. Harvey, D. Schröder, W. Koch, D. Danovich, S. Shaik, H. Schwarz

"Electron Transfer Reactivity in the Bond Activation of Organic Fluorides by Calcium Monocation"

Chem. Phys. Lett., **278**, 391−397 (1997), *Erratum in Full*

• A. Shurki, S. Shaik

"The Distortive Tendency of Benzene π-Electrons: How is it Related to Observables?"

Angew. Chem., Int. Ed., **36**, 2205−2208 (1997).

• A. Shurki, S. Shaik

"The Distortive Tendency of Benzene π-Electrons: How is it Related to Observables?"

Angew. Chem., **109**, 2322−2324 (1997).

• G.N. Sastry, S. Shaik

"A Theoretical Study of Electron Transfer and Substitution Mechanisms of Cyanoformaldehyde Anion Radical and Alkyl Halides: The Role of Steric Hindrance"

J. Am. Chem. Soc., **120**, 2131−2145 (1998).

• S. Shaik, M. Filatov, D. Schröder, H. Schwarz

"Electronic Structure Makes a Difference: Cytochrome P-450 Hydroxylation of Hydrocarbons as a Two-State Reactivity"

Chem. Eur. J., **4**, 193−199 (1998).

• An Electronic Publication:

D. Danovich, S. Shaik

"Ionization Energies and Electron Affinities of Fullerenes"

http://yfaat.ch.huji.ac.il/c60art.html

• 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.

• D. Danovich, C.M. Marian, T. Neuheuser, S.D. Peyerimhoff, S. Shaik

"Spin Orbit Coupling Patterns Induced by Twist and Pyramidalization Modes in C_2H_4:

A Quantitative Study and Qualitative Analysis"

J. Phys. Chem. A, **102**, 5923−5936 (1998).

• A. Shurki, S. Shaik

"The Perfectly Resonating State. A Chemical Model for the Transition State."

J. Mol. Struct. (THEOCHEM), **424**, 37−45 (1998).

The Lionel Salem Festschrieft Issue

• J.P. Dinnocenzo, M. Merchán, B.O. Roos, S. Shaik, H. Zuilhof

"Theoretical Study of the Electronic Spectra of Phenylcyclopropane and Cumene Cation

Radicals: Interplay of Experiment and Theory"

J. Phys. Chem. A, **102**, 8979−8987 (1998).

• 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).

• S. Grimme, M. Woeller, S.D. Peyerimhoff, D. Danovich, S. Shaik

"Theoretical Study of the Radationless Decay Channels of Triplet State Norbornene"

Chem Phys. Lett., **287** 601−607 (1998).

• S. Zilberg, Y. Haas, D. Danovich, S. Shaik

"The Twin Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibillvalene Rearrangement"

Angew Chem., Int. Ed., **37**, 1394−1397 (1998).

• S. Zilberg, Y. Haas, D. Danovich, S. Shaik

"The Twin Excited State as a Probe for the Transition State in Concerted Unimolecular Reactions: The Semibillvalene Rearrangement"

Angew. Chem., **110**, 1470−1473 (1998).

• M. Filatov, S. Shaik

"Spin Restricted Density Functional Approach to Open Shell Systems"

Chem. Phys. Lett., **288**, 689−697 (1998).

• W. Wu, S.-J. Zhong, S. Shaik

"VBDFT(s): A Hückel-type Semi-empirical Valence Bond (VB) Method Scaled to Density Functional Energies. Application to Linear Polyenes"

Chem. Phys. Lett., **292**, 7−14 (1998).

• S. Shaik, A. Shurki

"Valence Bond Diagrams and Chemical Reactivity"

Angew. Chem., Int. Ed., **38**, 586−625 (1999).

• S. Shaik, A. Shurki

"Valence Bond Diagrams and Chemical Reactivity"

Angew. Chem. **111**, 616−657 (1999).

• D. Danovich, W. Wu, S. Shaik

"No-Pair Bonding in the High-Spin $^3\Sigma_u^+$ State of Li_2. A Valence Bond Study of its Origins"

J. Am. Chem. Soc., **121**, 3165−3174 (1999).

• A. Shurki, P.C. Hiberty, S. Shaik

"Charge-Shift Bonding in Group IVB Halides: A Valence Bond Study of H_3M-Cl (M = C, Si, Ge, Sn, Pb) Molecules"

J. Am. Chem. Soc., **121**, 822−834 (1999); **121**, 9768 (1999) (Errata).

• M. Filatov, N. Harris, S. Shaik

"A Theoretical Study of Electronic Factors Affecting Hydroxylation by Model Ferryl Complexes of Cytochrome P-450 and Horse-Radish Peroxidase"

J. Chem. Soc., Perkin Trans., 2, 399−411 (1999).

• 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).

• N. Harris, W. Wu, W.H. Saunders, Jr., S. Shaik

"Origins of Nonperfect 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).

• 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).

• M. Filatov, S. Shaik

"An Ensemble-Referenced Kohn-Sham (ERKS) Method and Its Application to Diradicaloid Situations"

Chem. Phys. Lett., **304**, 429−437 (1999).

• M. Filatov, S. Shaik

"Tetramethylene Ethane (TME) Diradical: Experiment and Density Functional Theory Reach and Agreement"

J. Phys. Chem. A, **103**, 8885−8889 (1999).

• N. Harris, S. Shaik, D. Schröder, H. Schwarz

"Single- and Two-State Reactivity in the Gas Phase Activation of Norbornane by 'Bare' FeO^+"

Helv. Chem. Acta, **82**, 1784−1797 (1999).

• M. Filatov, N. Harris, S. Shaik

"On the 'Rebound' Mechanism of Alkane Hydroxylation by Cytochrome P-450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step"

Angew. Chem., Int. Ed., **38**, 3510−3512 (1999)

• M. Filatov, N. Harris, S. Shaik

"On the 'Rebound′ Mechanism of Alkane Hydroxylation by Cytochrome P-450: Electronic Structure of the Intermediate and the Electron Transfer Character in the Rebound Step"

Angew. Chem. **111**, 3730−3733 (1999)

• J.M. Galbraith, A. Shurki, S. Shaik

"A Valence Bond Study of Bonding in First Row Transition Metal Hydride Cations. What Energetic Role Does Covalency Play?"

J. Chem. Phys. A, **104**, 1262−1270 (2000).

• M. Woeller, S. Grimme, S.D. Peyerimhoff, D. Danovich, M. Filatov, S. Shaik

"A Theoretical Study of the Triplet State Radiationless Decay Mechanisms of Cyclic Olefins"

J. Phys. Chem. A, **104**, 5366−5373 (2000).

• 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).

• M. Filatov, S. Shaik, M. Woeller, S. Grimme, S.D. Peyerimhoff

"Locked Olefins with a Short Triplet State's Lifetime"

Chem. Phys. Lett., **316**, 135−140 (2000).

• 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 Energies, and NICS Values"

Chem. Eur. J., **6**, 1446−1454 (2000).

• 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 Lifetime"

Angew. Chem., Int. Ed., **39**, 2003−2007 (2000).

• 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, **79**, 92−123 (2000).

• D. Schröder, S. Shaik, H. Schwarz,

"Two-State Reactivity as a new Concept in Organometallic Chemistry"

Acc. Chem. Res., **33**, 139−145 (2000).

• 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).

• M. Filatov, S. Shaik

"Diradicaloids: Description by the Spin-Restricted Ensemble-Referenced Kohn-Sham (REKS) Density Functional Method"

J. Phys. Chem. A, **104**, 6628−6636 (2000).

• 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).

• F. Ogliaro, N. Harris, S. Cohen, M. Filatov, S.P. de Visser, S. Shaik

"A Model 'Rebound' Mechanism of Methane Hydroxylation by Cytochrome P450: Stepwise and Effectively Concerted Pathways and their Reactivity Patterns"

J. Am. Chem. Soc., **122**, 8977−8989 (2000).

• 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).

• M. Filatov, W. Reickien, S.D. Peyerimhoff, S. Shaik

"Why is the Mixture of H_2 and Oxygen O_2 Kinetically Stable?"

J. Phys. Chem. A, **104**, 12014−12020 (2000).

• F. Ogliaro, S. Cohen, M. Filatov, N. Harris, S. Shaik

"The High-valent Compound I of Cytochrome P450: The Nature of the Fe−S Bond and the Role of the Thiolate Ligand as Internal Electron Donor"

Angew. Chem., Int. Ed., **39**, 3851−3855 (2000).

• F. Ogliaro, S. Cohen, M. Filatov, N. Harris, S. Shaik

"The High-valent Compound I of Cytochrome P450: The Nature of the Fe−S Bond and the Role of the Thiolate Ligand as Internal Electron Donor"

Angew. Chem., **122**, 4009−4013 (2000).

• 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).

• 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).

• 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 It Really Is?"

J. Am. Chem. Soc., **122**, 12892−12893 (2000).

• S.P. de Visser, Y. Alpert, D. Danovich, S. Shaik

"No-Pair Bonding in High-Spin Lithium Clusters: $^{n+1}$Lin (n =2−6)"

J. Phys. Chem. A, **104**, 11223−11231 (2000).

• M. Filatov, S. Shaik

"Artificial Symmetry Breaking in Radicals Is Avoided by the Use of the REKS Method"

Chem. Phys. Lett., **332**, 409−419 (2000).

• S.P. de Visser, M. Filatov, S. Shaik

"REKS Calculations on *ortho- meta-* and *para*-Benzyne"

Phys. Chem. Chem. Phys., **2**, 5046−5048 (2000).

• 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)

• 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).

• 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**, 1501−1539 (2001).

• S. Shaik, W. Wu, K. Dong, L. Song, P.C. Hiberty

"Identity Hydrogen Abstraction Reactions, X• + H-X′ → XH + X′• (X = X′ = CH_3, SiH_3, GeH_3, SnH_3, PbH_3): A Valence Bond Modeling"

J. Phys. Chem. A, **105**, 8226−8235 (2001).

• 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).

• 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).

• 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).

• 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).

• 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).

• 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).

• S. Shaik

"Chemical Reactivity and Valence Bond Diagrams: A Personal Account"

Chem. Isr., **6**, 4−11 (2001).

• 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).

• BOOK

P.C. Hiberty, S. Shaik

"*BOVB- A Valence Bond Method Incorporating Static and Dynamic Correlation Effects"*

Valence Bond Theory. Theoretical and Computational Chemistry, in: "Valence Bond Theory"

D.L. Copper, D.J. Klein, Eds.

Elsevier Publications, NY, 2002, *Chapter* 7, pp 187−225.

• F. Ogliaro, S.P. de Visser, S. Cohen. J. Kaneti, S. Shaik

"The Experimentally Elusive Oxidant of Cytochrome P450: A Theoretical 'Trapping' Aiming Closer to the 'Real' Species"

ChemBioChem, **2**, 848−851 (2001).

• 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).

• 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).

• 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).

• 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).

• W. Wu, S. Shaik, W.H. Saunders, Jr.

"A Comparative Study of Identity Proton Transfer Reactions Between Simple Atoms and Groups by VBSCF Methods"

J. Phys. Chem. A, **106**, 11616−11622 (2002).

• L. Song, W. Wu, K. Dong, P.C. Hiberty, S. Shaik

"Valence Bond Modeling of Barriers in the Nonidentity Hydrogen Abstraction Reactions,

$X'\bullet + H\text{-}X \rightarrow X'H + X\bullet$ ($X \neq X' = CH_3$, SiH_3, GeH_3, SnH_3, PbH_3)"

J. Phys. Chem. A, **106**, 11361−11370 (2002).

• S. P. de Visser, D. Danovich, W. Wu, S. Shaik

"Ferromagnetic Bonds: Properties of "No-pair" Bonded High-Spin Lithium Clusters; $^{N+1}Li_N$ ($N = 2-12$)"

J. Phys. Chem. A, **106**, 4961−4969 (2002).

• S.P. de Visser, F. Ogliaro, S. Shaik

"Can Stereospecific Epoxidation by Compound I of Cytochrome P450 Proceed in a Concerted Synchronous Manner?"

J. Chem. Soc., Chem. Commun., 2322−2323 (2002).

• P.C. Hiberty, S. Shaik

"BOVB- A Modern Valence Bond Theory that Includes Dynamic Correlation"

Theor. Chem. Acc., **108**, 255−275 (2002).

• 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).

• S.P. de Visser, F. Ogliaro, P.K. Sharma, S. Shaik

"Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: A Chameleon Oxidant Behavior by Compound I"

Angew. Chem., Int. Ed., **41**, 1947−1951 (2002).

• W. Wu, L. Song, Z. Cao, Q. Zhang, S. Shaik

"VBCI: A Practical Valence Bond Method Incorporating Dynamic Correlation"

J. Phys. Chem. A, **106**, 2721−2726 (2002).

• F. Ogliaro, S.P. de Visser, S. Shaik

"The 'Push' Effect of Thiolate Ligands in Cytochrome P450: A Theoretical Gauging"

J. Inorg. Biochem., **91**, 554−567 (2002).

• S. Shaik, S.P. de Visser, W. Wu, L. Song, P.C. Hiberty

"Reply to Comment on: "Identity Hydrogen Abstraction Reactions, $X\bullet + H\text{-}X' \rightarrow XH + X'\bullet$ ($X = X' = CH_3$, SiH_3, GeH_3, SnH_3, PbH_3): A Valence Bond Modeling"

J. Phys. Chem. A, **106**, 5043−5045 (2002).

• 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).

• 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) (an electronic journal http://www.mdpi.org/ijms/)

• 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).

• S. Shaik, F. Ogliaro, S.P. de Visser, H. Schwarz, D. Schröder

"Two State Reactivity (TSR) Mechanism of Hydroxylation and Epoxidation by Cytochrome P450 Revealed by Theory"

Curr. Opin. Chem. Biol., **6**, 556−567 (2002).

• 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).
• S.P. de Visser, J. Kaneti, R. Neumann, S. Shaik
"Olefin Epoxidation by H_2O_2 is Accelerated by Fluorinated Alcohols: Template Catalysis"
J. Org. Chem., **68**, 2903−2912 (2003).
• A. Shurki, P.C. Hiberty, F. Dijkstra, S. Shaik
"Aromaticity and Antiaromaticity: What Role do Ionic Configuration Play in Delocalization and Induction of Magnetic Properties?"
J. Phys. Org. Chem., **16**, 731−745 (2003).
• S. Shaik, P.C. Hiberty
"Myth and Reality in the Attitude Toward Valence Bond (VB) Theory: Are Its Failures Real?"
Helv. Chim. Acta, **86**, 1063−1083 (2003).
• S. Shaik
"Chemistry- A Central Pillar of Human Culture"
Angew. Chem., Int. Ed., **42**, 3208−3215 (2003).
• S. Shaik
"Die Chemie − eine zentrale Saule der menschlichen Kultur"
Angew. Chem., **115**, 3326−3333 (2003).
• S.P. de Visser, M. Filatov, P.R. Schreiner, S. Shaik
"A REKS Assessment of the Face-Diagonal Bond in 1,3-Dihydrocubane and Comparison with Benzyme Radicals"
Eur. J. Org. Chem., 4199−4204 (2003).
• P.K. Sharma, S.P. de Visser, F. Ogliaro, S. Cohen and 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., **124**, 2291−2300 (2003).
• P.K. Sharma, S.P. de Visser, S. Shaik
"Can a Single Oxidant with Two Spin-States Masquerade as Two Oxidants?"
J. Am. Chem. Soc., **125**, 8698−8699 (2003).
• L. Song, W. Wu, P.C. Hiberty, D. Danovich, S. Shaik
"An Accurate Barrier for the Hydrogen Exchange Reaction from Valence Bond Theory: Is Valence Bond Theory Coming of Age?"
Chem. Eur. J., **9**, 4540−4547 (2003).
• 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).
• 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).
• S.P. de Visser, S. Shaik, P.K. Sharma, D. Kumar, W. Thiel
"The Active Species of Horse Radish Peroxidase (HRP) and Cytochrome P450: Two Electronic Chameleons"
J. Am. Chem. Soc. **125**, 15779−15788 (2003).
• P.K. Sharma, S. Shaik
"Science: Viewing La Vega" (Web site review)
Angew. Chem., Int. Ed., **42**, 968−969 (2003)
• R. Hoffmann, S. Shaik, P.C. Hiberty
"Conversation on VB vs. MO Theory: A Never Ending Rivalry?"
Acc. Chem. Res., **36**, 750−756 (2003).
• 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.
• 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).
• 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 Reactivity"
J. Inorg. Biochem., **98**, 1183−1193 (2004).
• 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).
• 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., **42**, 5661−5665 (2004).
• J.C. Schöneboom, S. Cohen, H. Lin, S. Shaik, W. Thiel
"QM/MM Investigation of the Mechanism of C−H Hydroxylation of Camphor by Cytochrome P450cam: Theory Supports a Two-State Rebound Mechanism"
J. Am. Chem. Soc., **126**, 4017−4034 (2004).
• J. Li, X. Li, S. Shaik, H.B. Schlegel
"A single Transition State Serves Two Mechanisms. Ab Initio Classical Trajectory Calculations of the Substitution-Electron Transfer Branching Ratio of $CH_2O^{-}\bullet + CH_3Cl$"
J. Phys. Chem. A, **108**, 8526−8532 (2004).
• 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 Mono-Oxygenations by Cytochrome P450"
Eur. J. Inorg. Chem., 207−226 (2004).
• S. Shaik, P.C. Hiberty
"*Valence Bond Theory, Its History, Fundamentals and Applications- A Primer*"
Rev. Comput. Chem., **20**, 1−100 (2004).
• 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).
• 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).
• S. Kozuch, S. Shaik, A. Jutand, C. Amatore
"Active Zero-Valent Palladium Catalysts: Characterization by Density Functional Calculations"
Chem. Eur. J., **10**, 3072−3080 (2004).
• P.K. Sharma, R. Kevorkiants, 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**, 1149−1152 (2004).

• P.K. Sharma, R. Kevorkiants, S.P. de Visser, D. Kumar, and S. Shaik

"Porphyrin Traps its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450"

Angew. Chem. **116**, 1129−1132 (2004).

• H. Lin, J.C. Schöneboom, S. Cohen, S. Shaik, W. Thiel

"QM/MM Study of the Product Enzyme Complex in P450cam Catalysis"

J. Phys. Chem. B, **108**, 10083−10088 (2004).

• 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

DOI: 10.1002/0470845015.cu0017, online edition. http://www.mrw.interscience.wiley.com/ecc/articles/cu0017/abstract-fs.html

• B. Meunier, S.P. de Visser, S. Shaik

"Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes"

Chem. Rev., **104**, 3947−3980 (2004).

• P.C. Hiberty, S. Shaik

"The Distortive Tendencies of π-Electronic Systems, the Relationship to Isoelectronic σ-Bonded Analogs, and Observables: A Unified Description Free of the Classical Paradoxes"

Phys. Chem. Chem. Phys., **6**, 224−231 (2004).

• 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 it Normal Function?"

J. Am. Chem. Soc., **126**, 5072−5073 (2004)

• 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).

• S. Shaik, S.P. de Visser, D. Kumar,

"An External Electric Field Will Control the Selectivity of Enzymatic-Like Bond Activations"

J. Am. Chem. Soc., **126**, 11746−11749 (2004)

• S. Shaik, S.P. de Visser, D. Kumar

"One Oxidant, Many Pathways: A Theoretical Perspective of Monoxygenation Mechanisms by Cytochrome P450"

J. Biol. Inorg. Chem., **9**, 661−668 (2004).

• 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).

• 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).

• C. Amatore, A. Jutand, F. Lemaître, 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).

• S. Shaik, D. Danovich, B. Silvi, D. 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).

• 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.

• S. Kozuch, T. Leifels, S. Shaik, W.-D. Woggon

"New Synthetic Models of Cytochrome P450: How Different are they from the Natural Species?"

SynLett., **4**, 675−684 (2005).

• D. Kumar, S.P. de Visser, P.K. Sharma, E. Derat, S. Shaik

"The Axial Ligand Effect on Propene Oxidation by Horseradish Peroxidase vs Cytochrome P450 Enzymes"

J. Biol. Inorg. Chem., **10**, 181−189 (2005).

• S. Shaik, P.C. Hiberty

"A 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

• D. Kumar, S.P. de Visser, S. Shaik

"Theory Favors Stepwise Mechanism of Porphyrin Degradation by a Ferric Hydroxperoxide Model Species of Heme Oxygenase"

J. Am. Chem. Soc., **127**, 8204−8213 (2005).

• 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).

• D. Kumar, S.P. de Visser, S. Shaik

"Multi-State reactivity in the Epoxidation of Styrene by Compound I of Cytochrome P450: Mechanisms of Products and Side Products Formation"

Chem Eur. J., **11**, 2825−2835 (2005).

• S. Shaik, S.P. de Visser, D. Kumar, A. Altun, W. Thiel,

"Theoretical Perspective on Structure and Mechanisms of Cytochrome P450 Enzymes"

Chem. Rev., **105**, 2279−2328 (2005).

• P.C. Hiberty, S. Shaik

"Some Frequently Asked Questions About the Distortive Tendencies of π-Electronic Systems"

Theor. Chem. Acc., **114**, 169−181 (2005).

• D. Kumar, H. Hirao, L. Que, Jr., S. Shaik

"Theoretical Investigation of C−H Hydroxylation by $(N_4Py)Fe^{IV}{=}O^{2+}$: An Oxidant More Powerful than P450?"

J. Am. Chem. Soc., **127**, 8026−8027 (2005).

• S. Kozuch, A. Jutand, C. Amatore, S. Shaik

" What Makes for a Good Catalytic Cycle? A Theoretical Study of the Role of Anionic Pd(0) in the Cross-Coupling Reaction of An Aryl Halide with a Nucleophile"

Organometallics, **24**, 2319−2330 (2005).

• 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 Formation of Compound I from Compound 0"

J. Phys. Chem. B, **109**, 19946−19951 (2005).

• 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).

• 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).

• 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).

• W. Wu, W.H. Saunders, S. Shaik

"VB Calculations for the E2 Reaction of Fluoride ion with Ethyl Fluoride. Implications for the More O'Ferrall-Jencks Diagram"

Can. J. Chem., **83**, 1649−1653 (2006).

• L. Song, W. Wu, P.C. Hiberty, S. Shaik

"The Identity S_N2 Reaction $X^- + CH_3\text{-}X \rightarrow X\text{-}CH_3 + X^-$ in the Gas Phase and in Solution: A Valence Bond Study"

Chem. Eur. J., **12**, 7458−7466 (2006).

• A. Altun, S. Shaik, W. Thiel

"Systematic QM/MM Investigation of Factors that Affect the Cytochrome $P450_{cam}$ − Catalyzed Hydrogen Abstraction of Camphor"

J. Comput. Chem., **27**, 1324−1337 (2006).

• 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).

• 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).

• 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).

• 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).

• S. Shaik

"A Tale of Two States", pp 233−249.

In "*Modeling Molecular Structure and Reactivity in Biological Systems*"

K.J. Naidoo, J. Brady, M.J. Field, J. Gao, M. Hann, Eds.

RSC Publishing, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 0WF, UK, 2006

• H. Hirao, D. Kumar, L. Que, Jr., S. Shaik

"Two-State Reactivity in C−H Hydroxylation by Non-Heme Iron Oxo Complexes"

J. Am. Chem. Soc., **128**, 8590−8606 (2006).

• 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).

• A. Altun, R.A. Friesner, V. Guallar, S. Shaik, W. Thiel,

"The Effect of Heme Environment on the Hydrogen Abstraction of Camphor in P450cam Catalysis: A QM/MM Study"

J. Am. Chem. Soc., **128**, 3924−3925 (2006).

• D. Kumar, H. Hirao, S. Shaik, P.M. Koslowski

"A Proton-Shuffle Mechanism of O−O Activation for the Formation of the High-Valent Oxo-Iron Species of Bleomycin"

J. Am. Chem. Soc., **128**, 16148−16158 (2006).

• 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 Probe Substrate"

J. Am. Chem. Soc., **128**, 473−484 (2006).

• 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).

• 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).

• H. Hirao, S. Shaik, P.M. Koslowski

"Theoretical Analysis of Structural and Electronic Properties of Metalloporphyrin π-Cation Radicals"

J. Phys. Chem. A, **110**, 6091−6099 (2006).

• E. Derat, S. Shaik

"Two-state Reactivity, Electromerism, Tautomerism and 'Surprise' 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).

• 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).

• J. Li, S. Shaik, H.B. Schlegel

"A Single Transition State Serves Two Mechanisms. The Branching Ratio for $CH_2O^{-\bullet} + CH_3Cl$ on Improved Potential Energy Surface"

J. Phys. Chem. A, **110**, 2801−2806 (2006).

• E. Derat, D. Kumar, R. Neumann, S. Shaik

"Seeking for New Robust Catalysts for Monooxygenations Made From Polyoxometalate: An Iron-Oxo Derivative of the Lindqvist Anion"

Inorg. Chem., **45**, 8655−8663 (2006).

• A.M. Khnekin, D. Kumar, S. Shaik, R. Neumann

"Characterization of Mn(V) Oxo Polyoxometalate Intermediates and their Properties in Oxygen Transfer Reactions"

J. Am. Chem. Soc., **128**, 15451−15460 (2006).

• 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).

• 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).

• 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**, 13204−13214 (2006).

• 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-Methylenenylcamphor"

J. Inorg. Biochem., **100**, 2054−2068 (2006).

• S. Shaik

"Is My Chemical Universe Localized or Delocalized? Is there a Future For Chemical Concepts?"

New. J. Chem., **31**, 2015−2028 (2007).

• P. Su, L. Song, W. Wu, P.C. Hiberty, S. Shaik

"The Dioxygen Molecule: A Valence Bond Description of a Historically Enigmatic Molecule"

J. Comput. Chem., **28**, 185−197 (2007).

• S. Shaik

"The Lewis Legacy − The Chemical Bond; A Territory and Heartland of Chemistry"

J. Comput. Chem., **28**, 51−61 (2007).

• C. Hazan, D. Kumar, S.P. de Visser, S. Shaik

" A Density Functional Study of the Factors that Influence the Chemoselectivity of Toluene Hydroxylation by Cytochrome P450 Enzymes"

Eur. J. Inorg. Chem., 2966−2974 (2007).

• G. Frenking, S. Shaik

Foreword to the Issue "90 Years to the Lewis Concept"

J. Comput. Chem., **28**, 1−3 (2007).

• P.C. Hiberty, S. Shaik

"Some Recent Developments of *Ab Initio* Valence Bond Theory"

J. Comput. Chem., **28**, 137−151 (2007).

• BOOK

S. Shaik, P.C. Hiberty

"*A Chemist's Guide to VB Theory*"

Wiley-Interscience, 2007.

• P. Su, F. Ying, W. Wu, P.C. Hiberty, S. Shaik

"The Menshutkin S_N2 Reaction $H_3N + CH_3Cl - H_3HCH_3^+ + Cl^-$: A VBPCM Study"

ChemPhysChem, **8**, 2603−2614 (2007).

• K. Kühnel, E. Derat, J. Terner, 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).

• 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).

• S. Shaik, H. Hirao, D. Kumar

"Reactivity Patterns of Cytochrome P450- Multi-State Functionality of the Active Species and the Two States-Two Oxidants Conundrum"

Nat. Prod. Rep., **24**, 533−552 (2007).

• D. Fishelovitch, C. Hazan, H. Hirao, H.J. Wolfson, R. Nussinov, S. Shaik

"A QM/MM Study of the Active Species of the Human P450 3A4, and the Influence Thereof of the Cooperative Binding of Substrates"

J. Phys. Chem. B, **111**, 13822−13832 (2007).

• Y. Wang, K. Han, S. Shaik

"A New Mechanism of Ethanol Oxidation by CYP2E1"

ChemBioChem, **8**, 277−281 (2007).

• Y. Wang, D. Kumar, C. Yang, H. Wang, K. Han, S. Shaik

"A Theoretical Study of the Mechanism of Cytochrome P450-Catalyzed Demthylation of *N,N*-dimethylanilines"

J. Phys. Chem. B, **117**, 7700−7710 (2007).

• 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 Tunes the Reactivity?"

J. Phys. Chem. B, **111**, 10288−10299 (2007).

• P.C. Hiberty, R. Ramozzi, L. Song, W. Wu, S. Shaik

"The Physical Origins of Large Covalent-Ionic Resonance Energies in Some Two-Electron Bonds"

Faraday Discuss., **135**, 261−272 (2007).

• 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 Induced by Electron Transfer"

J. Phys. Chem. C, **111**, 7711−7719 (2007).

• K.-B. Cho, E. Derat, S. Shaik

"The Compound I Species of Nitric Oxide Synthase Synthase: The Active Site Protonation State"

J. Am. Chem. Soc., **129**, 3182−3188 (2007).

• 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 HRP"

J. Am. Chem. Soc., **129**, 6346−6347 (2007).

• 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).

• D. Fishelovitch, S. Shaik, H.J. Wolfson, R. Nussinov

"Structural Dynamics of the Cooperative binding of Organic Molecules by Human Cytochrome P450 (Cyp450) 3A4"

J. Am. Chem. Soc., **129**, 1602−1611 (2007).

• A. Altun, S. Shaik, W. Thiel

"QM/MM Studies of Camphor Hydroxylation by Cytochrome P450 for Different Electronic States of Compound I and Related Intermediates"

J. Am. Chem. Soc., **129**, 8978−8987 (2007).

• C. Li, L. Zhang, C. Zhang, W. Wu, H. Hirao, S. Shaik

"Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?"

Angew. Chem., Int. Ed., **46**, 8168−8170 (2007).

• 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).

• 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).

• P. Su, L. Song, W. Wu, S. Shaik, P.C. Hiberty

"Heterolytic Bond Dissociation in Water: Why So Easy for C_4H_9Cl But Not for C_3H_9SiCl?"

J. Phys. Chem. A, **112**, 2988−2997 (2008).

• 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).

• 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).

• H. Hirao, L. Que, Jr., W. Nam, S. Shaik

"A TSR Rationale for the Counterintuitive Axial Ligand Effect on the C−H Activation Reactivity of Nonheme Fe(IV)═O Oxidants"

Chem. Eur. J., **14**, 1740−1756 (2008).

• H. Chen, Y. Moreau, E. Derat, S. Shaik

"QM/MM 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).

• D. Wang, J. Zheng, W. Thiel, S. Shaik

"QM/MM Study of the First Proton Transfer in the Catalytic Cycle of Cytochrome P450cam and its Mutant D251N"

J. Phys. Chem. B, **112**, 5126−5138 (2008).

• 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).

• 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).

• P. Su, W. Wu, S. Shaik, P.C. Hiberty

"A Valence Bond Study of Low-Lying States of the NF Molecule"

Chem. Phys. Chem., in press.

• H. Chen, H. Hirao, E. Derat, I. Schlichting, S. Shaik

"Quantum Mechanical/Molecular Mechanical Study on Mechanisms of Compound I Formation in the Catalytic Cycle of Chloroperoxidase − An Overview on Heme Enzymes"

J. Phys. Chem. B, **112**, 9490−9500 (2008).

• S. Kozuch, S. Shaik

"A 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).

• 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"

J. Am. Chem. Soc., **112**, 10128−10140 (2008); **112**, 14016 (2008) (Correction).

• H. Chen, M. Ikeda-Saita, S. Shaik

"The Nature of the Fe–O_2 Bonding in Oxy–Myoglobin - The Effect of the Protein"

J. Am. Chem. Soc., **112**, ASAP (2008) (DOI: 10.1021/ja805434m).

JP806628J