Curriculum Vitae Dr. David Danovich

14 January 2021
(h-index: 34; 124 publications)

Personal Information

Name:
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Date of Birth:
June 29, 1959

Place of Birth:
Irkutsk, USSR

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Contact information

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Current position

1992- present: Senior computational chemist and scientific programmer in the Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

Scientific skills

Very experienced scientific researcher with demonstrated ability to implement *ab initio* molecular electronic structure and valence bond calculations for obtaining insights into physical and chemical properties of molecules and materials.
Extensive expertise in implementation of Molecular Orbital Theory based on *ab initio* methods such as Hartree-Fock theory (**HF**), Density Functional Theory (**DFT**), Moller-Plesset Perturbation theory (**MP2-MP5**), Couple Cluster theories [**CCST(T)**], Complete Active Space (**CAS, CASPT2**) theories, Multireference Configuration Interaction (**MRCI**) theory and modern *ab initio* valence bond theory (**VBT**) methods such as Valence Bond Self Consistent Field theory (**VBSCF**), Breathing Orbital Valence Bond **theory** (**BOVB**) and its variants (like **D-BOVB**, **S-BOVB** and **SD-BOVB**), Valence Bond Configuration Interaction theory (**VBCI**), Valence Bond Perturbation theory (**VBPT**).

Language skills

Advanced
English, Russian

Conversational
Hebrew

Academic background

1. *Undergraduate studies, 1978-1982*
Master of Science in Physics, June 1982
Irkutsk State University, USSR

2. *Graduate studies, 1984-1989*
Ph. D. in Quantum Chemistry, May 1989
Irkutsk State University, USSR.
Supervisors: Prof. V.K. Voronov and Dr. V.G. Zakrzewskii
Title of the thesis: **"Quantum Chemical Investigation of the Electronic Structure of the 1-vinylazoles and Their Complexes "**

3. *Post-doctoral employment, 1990-1992*
Post-doctoral fellow, July 1990 - July 1992
Supervisor: Prof. Yitzhak Apeloig, Department of Chemistry, Technion-Israel Institute of Technology, Haifa, Israel

Programmer skills

Extensive LINUX system administrating experience on **RedHat (CentOS)** and **Ubuntu** operation systems as well as on Windows 10 and Mac OS X operation systems.
Programming skills with Fortran, Mathematica, Javascript, UNIX shell script, HTML, etc in various degrees.

Computational skills

Extensive experience of installing, implementing, interfacing and using a range of highly ranked computational chemistry software like **Gaussian, Jaguar, MOLCAS, MOLPRO, GAMESS-US, ORCA, NWChem, QChem, Turbomole, Dalton, XMVB, MOPAC, ELF, GROMACS, POLYRATE, DL-POLY, CHARMm** etc. on **Linux** operation system**.**

References (The following persons have agreed to provide reference letter upon request)

Prof. Sason Shaik
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Presentation at Conferences and Symposia

[1] 10th IUPAC Conference on Physical Organic Chemistry. Technion, Haifa, Israel, August 5-10, 1990, Abstract PO-B-17. (Poster presentation)

D. Danovich. "**Influence of the type and position of a substituent on the orbital structure of 2-, 3- and 4- substituted pyridines. OVGF(AM1) data**"

[2] 10th IUPAC Conference on Physical Organic Chemistry. Technion, Haifa, Israel, August 5-10, 1990, Abstract PO-B-18. (Poster presentation)
D. Danovich and V.K.Turchaninov. "**Basicity of nitrogen heterocycles. Relationship with the energy of their nonbonding electrons and with the energy of electronic reorganization upon ionization**"

[3] Chemistry on the InfoBahn (electronic poster), 210th ACS National meeting, Chicago, August 20-24, 1995, Division of Computers in Chemistry, poster 35. (Electronic poster presentation)
D. Danovich and S. Shaik. "**Ionization potentials and electron affinities of fullerenes. An OVGF approach**"

[4] Molecular Quantum Mechanics: Methods and Applications. An International Conference in memory of Samuel Francis Boys and in honor of Isaiah Shavitt. University of Cambridge, England, 3-7 September, 1995, Poster C-21. (Poster presentation)
D. Danovich and S. Shaik. "**Excited states of Li_2. CASPT2 and VBSCF approaches**"

[5] 211th American Chemical Society National Meeting, Division of Computers in Chemistry, "Semiempirical Methods: Is there a Future?", New Orleans, LA, March 24-28, 1996, paper 137. (Invited lecture)
D. Danovich. "**NDDO Semiempirical Approximations coupled with Green's Function Technique - a Reliable Approach for Calculating Ionization Potentials**"

[6] 4th World Congress of Theoretically Oriented Chemists-WATOC'96, Jerusalem, Israel, July 7-12, 1996. A-13. (Contributed lecture)
D. Danovich and S. Shaik. "**Origins of the bonding in high spin Li clusters. A valence bond study of $^3Li_2$ and $^4Li_3$**"

[7] 62nd Meeting of the Israel Chemical Society, Haifa, Israel, February 3-5, 1997, I52. (Invited lecture)
D. Danovich. "**Origins of the bonding in the triplet state of alkali metal dimmers. A valence bond study**"

[8] 66th Meeting of the Israel Chemical Society, Tel-Aviv, Israel, February 5-6, 2001. (Invited lecture)
D. Danovich, F. Ogliaro, M. Karni, Y. Apeloig, D.L. Cooper and Sason Shaik. "**Are C=Si and Si=Si bonds true triple bonds? A valence bond analysis**"

[9] 1th Theoretical Meeting of the Israel Chemical Society, Jerusalem, Israel, October 9-10, 2002. (Invited lecture)
D. Danovich "An initio Valence Bond – A reliable tool for describing the chemical bonds"

[10] 7th World Congress of Theoretically Oriented Chemists-WATOC'05, Cape Town, South Africa, January 16-21, 2005. (Contributed lecture).
D. Danovich and Sason Shaik. "**Triple bonds of Carbon and Silicon - A comparative study using modern valence bond theory**"

[11] Beirat Symposium of the Lise Maitner Minerva Center, Jerusalem, Israel June 17, 2007. (Invited lecture)
D. Danovich. "**Ferromagnetic bonding in high spin clusters of coinage metals**"

[12] 13th International Congress of Quantum Chemistry, Helsinki, Finland, June 22-27, 2009. (Poster presentation)
D. Danovich and S. Shaik. "**Investigation of the No-Pair Bonding in the High Spin States of the**

Coinage Metal Clusters Using Valence Bond, Density Functional and CCSD(T) methods"

[13] 9th World Congress of Theoretically Oriented Chemists-WATOC'11, Santiago de Compostella, Spain, July 18-23, 2011. (Poster presentation)
D. Danovich and S. Shaik. "**Triple bonds of Carbon and Silicon - A comparative study using modern valence bond theory**"

[14] 9th World Congress of Theoretically Oriented Chemists-WATOC'11, Satellite Conference on Highly Correlated Methods, Coruna, Spain, July 24-25, 2011. (Invited lecture)
D. Danovich and S. Shaik. "**Why the High Spin State of the Metal Clusters are Bound? Valence Bond Analyze of the No-Pair Bonding**"

[15] 30th Israel Vacuum Society meeting, Tel Aviv, Israel, October 15, 2012. (Contributed lecture).
D. Danovich. "**Ferromagnetic bonding in the highest spin states of monovalent metal clusters based on ab initio, DFT and valence bond analysis**"

[16] 10th World Congress of Theoretically Oriented Chemists-WATOC'14, Santiago, Chile, October 5-10, 2014. (Contributed lecture)
D. Danovich, C. Wang, Y. Mo and S. Shaik. "**Ab initio valence bond and block-localized wave function investigation of the Nature of the halogen bonds in the complexes of Lewis bases with dihalogens**"

[17] International conference "Chemical Bond in the 21 century", Xiamen, China, 14-18 June, 2015. (Contributed lecture)
D. Danovich, C. Wang, Y. Mo and S. Shaik. "**Ab initio valence bond and block-localized wave function investigation of the Nature of the halogen bonds in the complexes of Lewis bases with dihalogens**"

Lectures

1. August 1993, Theoretical Chemistry Group, University of Utrecht, The Netherlands
Title: "A Reliable and Inexpensive Method for Calculating Ionization Potentials and Electron Affinities of Radicals and Molecules"

2. December 1994, Institute für Organiche Chemie, Technische Universität Berlin, Germany
Title: "Outer Valence Green Function for Calculations of Ionization Potentials of Molecules"

3. December 1995, Institut für Physikalische und Theoretische Chemie der Universität Bonn, Bonn, Germany
Title: "Green's Function Method as a Reliable Approach for Calculating Ionization Potentials and Electron Affinities"

4. March 1996, Department of Physical Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "NDDO Semiempirical Approximations coupled with Green's Function Technique - a Reliable Approach for Calculating Ionization Potentials"

5. March 1996, Department of Chemistry, University of New Mexico, Albuquerque, New Mexico, USA.
Title: "NDDO Semiempirical Approximations coupled with Green's Function Technique - a Reliable Approach for Calculating Ionization Potentials"

6. April 1996, Department of Chemistry, University of Rochester, Rochester, New York, New York,

USA.
Title: "Origins of the bonding in high spin Li clusters. A valence bond study"

7. June 2001, Beirat Meeting, Institute of Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "A Valence Bond Description of the Triple Bonds Between Group 14 Elements"

8. October 2004, Beirat Meeting, Institute of Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "Triple bonds of carbon and silicon – a comparative study using modern valence bond theory"

9. June 17, 2007, Beirat Meeting, Institute of Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "Ferromagnetic bonding in the high spin states of coinage metal clusters"

10. December 10, 2009, Beirat Meeting, Institute of Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "No-pair bonding in the high-spin states of metal clusters"

11. June 27, 2010, Beirat Meeting, Institute of Chemistry, The Hebrew University, Jerusalem, Israel.
Title: "Ferromagnetic bonding in the high spin states of coinage metal clusters of Cu, Ag and Au"

Tutor at workshops

1. **25-28 September 2002**, Blankensee, Germany, Workshop: "Valence bond",
2. **16-20 July 2012**, Paris, France, Workshop: "Ab initio valence bond theory"
3. **14-18 June 2015**, Xiamen, China, Workshop: "Ab initio valence bond theory"

Organizing committees of symposia and meetings

1997-2017: Member of organizing committees of 18 Lise Meitner International Symposia of the Lise Meitner-Minerva Center for Computational Quantum Chemistry.

Summary of research achievements

(a) OVGF method: Developed a new approach for calculating ionization potentials of large molecules based on Green's function technique using semiempirical approximations. OVGF method allows correctly reproduce photoelectron spectrum of organic molecules.

New Bonding paradigms in collaboration with Prof. S. Shaik

(b) Charge-Shift Bonding (CSB): In addition to the classical covalent and ionic bonds, there exist a family of bonds that have never before been recognized. These are the charge-shift bonds (CSB) in which the binding does not arise from either the covalent- or the ionic-VB states, but from their resonance interaction (i.e. the coupling between the two VB states). We have shown that CSBs have experimental manifestations and the charge-shift resonance energy can even be quantified from experiments.
(c) The Triplet Bond - Bonding of Parallel Spins: We described no-pair ferromagnetic (NPFM) bonds that hold together monovalent metallic atoms using exclusively parallel spins. Thus, without any

traditional electron-pair-bonds, the bonding energy per two atoms in these clusters can nevertheless reach 40 kcal mol^{-1}! The VB modeling shows that this bonding motif arises from bound triplet electron pairs (hence may be called, the Triplet Bond) that are delocalized over all the close neighbors of a given atom in the cluster. The VB model shows the origins of the tendency of NPFM clusters to assume polyhedral shapes with rather high symmetry, and for the very steep rise of the bonding energy with cluster size. The advent of NPFM clusters offers new horizons in chemical bonding, and in chemistry of highly magnetic species, sensitive to magnetic and electric fields.

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

(e) Weak Intermolecular Interactions: We have developed VB-based models which lead to a lucid understanding of weak interactions such as dihydrogen interactions and halogen-bonds.

Developing of Quantum Chemistry Programs

1. D. Danovich, QCPE Bulletin, 11, N 2 (1991) 31, OVGF(SEMI): Molecular Orbital Package for Outer Valence Green's Function Calculations Coupled with the MNDO, MNDOC, AM1 and PM3 Semiempirical approximations, Indiana University, Bloomington IN 47405, USA.

2. D. Danovich, MOPAC 93, New Functionalities (MOPAC 93 Manual, p. 7), Fujitsu Limited, Japan.

a) Ionization potentials are corrected using Green's Function techniques. The resulting I.P.s is generally more accurate than the conventional I.P.s.
(http://www.cachesoftware.com/mopac/Mopac2002manual/node472.html)

b) The point-group of the system is identified, and molecular orbitals are characterized by irreducible representation. (http://www.cachesoftware.com/mopac/Mopac2002manual/node560.html)

3. D. Danovich, AMPAC 5.0-8.0, AMPAC Manual, SemiChem Inc., Kansas, USA
http://www.semichem.com/ampacmanual/contributors.html.

a) The point-group of the system is identified, and molecular orbitals are characterized by irreducible representation.

Research Interests and Current Research Activities

Chemical bonding - from small molecules to clusters.

1. Investigation of the mechanism of no-pair bonding which appears in high-spin alkali and coinage metals clusters, which are devoid of electron pairs but can still be strongly bonded.
2. “Charge-shift bonding” describes a mechanism of bonding which is neither covalent nor ionic, and which appears in homonuclear as well as heteronuclear bonds. We are trying to find now manifestations of this bonding type in chemistry of ground state molecules.
3. Investigation of bonding in the aluminium clusters. Such clusters can be used in nanotechnology.
4. Investigation of bonding in triply bonded silicon and carbon contains molecules.
5. Investigation of bonding in weakly bonded systems included halogen and hydrogen bonds.
6. Design and implementation of codes for quantum chemical computations and development of theoretical models for chemical systems.

List of publications

Google Scholar: h-index: 32; total citations: 3360. WEB of Science: h-index: 34, total citations: 2882. Total number of publications: 125; 5 invited chapters (publications 91, 96, 97, 107, 108) and 1 invited paper for Encyclopaedia of Computational Chemistry (publication 47).

[1] **D.K Danovich**, V.G. Zakrzewski, V.K.Voronov
Subroutine package for calculating molecular structures by the paramagnetic-additive method
Journal of Structural Chemistry, **27**, 320-321 (1986)

[2] **D.K. Danovich**, V.K. Voronov, V.G. Zakrzewski, E.S. Domnina
Quantum-chemical calculation of the geometry of 1-vinylazoles
Journal of Structural Chemistry, **27**, 658-659 (1986)

[3] A. Afonin, V.K. Voronov, M.A. Andriankov, **D.K. Danovich**
Structure of pyridine and quinoline vinyl ethers according to data from ^{1}H and ^{13}C NMR spectra and quantum-chemical calculations
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **36**, 279-284 (1987)

[4] **D.K. Danovich**, V.K. Voronov, V.G. Zakrzewski, L.A. Baikalova
Quantum-chemical study of the electronic structure and geometry of 1-vinylimidazole derivatives
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **36**, 1855-1857 (1987)

[5] **D.K. Danovich**, V. Zakrzewski, V. Voronov, E. Domnina, M. Voronkov
Computation of ionization energies from photoelectron spectroscopy data using the Green's function method in semiempirical AM1 approximation
Doklady of the Academy of Science of the USSR, **300**, 879-882 (1988)

[6] **D.K. Danovich**, V.K. Voronov, L.A. Es'kova
Quantum-chemical study of the electronic structure and geometry of 1-vinylpyrazole derivatives
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **37**, 278-283 (1988)

[7] A.V. Afonin, **D.K. Danovich**, V.K. Voronov, L.A. Es'kova, L.V. Baikalova, S.R. Buzilova
Analysis of the long-range effect of the nitrogen unshared pair on the direct ^{13}C-^{1}H coupling constants in the vinyl group of N-vinylazoles
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **37**, 752-755 (1988)

[8] A.V. Afonin, A.V. Vashchenko, **D.K. Danovich**, B.V. Trzhtsinskaya, L.V. Baikalova, E.V. Apakina
Enhancement of the direct 13C-1H coupling constant upon physical approximation of the proton and heteroatom in N-vinylheterocycles
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **38**, 1538-1541 (1989)

[9] **D.K. Danovich**, V.G. Zakrzewsky, V.K. Voronov, E.S. Domnina
Calculations of photoelectron spectra of azoles by the AM1 method using a Green's function approximation for outer valence molecular orbitals
Theoretical and Experimental Chemistry, **25**, 659-661 (1989)

[10] A.V. Afonin, A.V. Vashchenko, V.K. Voronov, **D.K. Danovich**, O.A. Zasyako
Quantum-chemical description of lone pairs of electrons of oxygen atom vinyl ethers
Journal of Organicheskoi Chemistry, **25**, 240-244 (1989)

[11] **D.K. Danovich**, V.K. Voronov, A.V. Afonin, E.S. Domnina, L.V. Baikalova, L.A. Es'kova
Study of hydrohalogenation of 1-vinylazoles by the MNDO method
Journal of General Chemistry, **59**, 651-657 (1989)

[12] **D.K. Danovich,** V.K. Turchaninov

Basicity of azoles. 1. Application of the method of partitioning of the total energy of pyrazole and imidazole derivatives
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **38**, 1182-1187 (1989)

[13] **D.K. Danovich,** V.K. Turchaninov.
Basicity of azoles. 2. Relationship with energy of nonbonding electrons and energy of reorganization of π- and σ- electron systems of a base in ionization and protonation
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **38**, 2480-2486 (1989)

[14] V.G Zakrzewski, **D.K. Danovich**
Realization of the Green's function method for calculations of PES based of the semiempirical approximations MNDO and AM1
Journal of Structural Chemistry, **30**, 474-477 (1989)

[15] **D.K. Danovich**, V.G. Zakrzewski, E.S. Domnina
AM1 outer valence Green's function ionizations energies of the azoles
Journal of Molecular Structure (Theochem), **187**, 297-306 (1989)

[16] **D.K Danovich**, V.G. Zakrzewski, E.S. Domnina
Ionization energies of azines from Green's function method in semiempirical AM1 approximation
Journal of Molecular Structure (Theochem), **188**, 159-166 (1989)

[17] A.V. Afonin, L.B. Krivdin, **D.K. Danovich**, V.K. Voronov, K.A. Es'kova, B.V. Trzhtsinskaya, L.V. Baikalova, S.R. Buzilova, G.A. Gareev
Direct ^{13}C-^{13}C spin-spin coupling constants in vinyl group of N-vinylazoles
Chemistry of Heterocyclic Compounds, **25**, 157-160 (1989)

[18] **D.K. Danovich**, B.N. Plakhutin, V.K. Voronov
The quantum-chemical study of the structure and isotropic chemical shifts in the NMR spectrum of the paramagnetic complex of 1-vinylimidazole with $CuCl_2$
Theoretical and Experimental Chemistry, **26**, 208-212 (1990)

[19] **D.K. Danovich**, V.K. Turchaninov, V.G. Zakrzewski
OVGF AM1 calculations of the ionization energies of pyridine derivatives
Journal of Molecular Structure (Theochem), **209**, 77-87 (1990)

[20] M.A. Fedotov, B.Z. Pertsikov, **D.K. Danovich**
^{17}O, ^{31}P and ^{183}W NMR spectra of paramagnetic complexes with the heteropolytungstate anion $[Ln(PW11O39)2]^{11-}$ and their constitution in aqueous solution. Ln--Rare earth element
Polyhedron, **9**, 1249-1256 (1990)

[21] A.V. Afonin, **D.K. Danovich**, V.K. Voronov, L.A. Es'kova, L.V. Baikalova, E.S. Domnina
Rotational-isomerism in 1-vinylpyrazoles and 1-vinylimidazoles according to ^{1}H, ^{13}C NMR and quantum chemical calculations
Chemistry of Heterocyclic Compounds, **26**, 1121-1125 (1990)

[22] A.V. Afonin, A.V. Vashchenko, **D.K. Danovich**
Study of the nature of the long-range effect of the lone pair of the heteroatom on the direct ^{13}C-^{1}H spin-spin coupling constants in N-vinyl derivatives of heterocycles by the AM-1 method
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **40**, 503-510 (1991)

[23] V.K. Turchaninov, **D.K. Danovich**, A.F. Ermikov, V.G. Zakzhevskii, L.A. Es'kova
Interpretaion of photoelectron spectra using the semiempirical AM1 method. I. Nitroazoles
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **40**, 2181-2184 (1991)

[24] H. U. Siehl, F. P. Kaufmann, Y. Apeloig, V. Braude, **D. Danovich,** A. Berndt, N. Stamatis
The observation of the first persistent β-silyl-substiuted vinyl cation
Angewante Chemie, International Edition English, **30**, 1479-1482 (1991)

[25] **D. Danovich,** Y. Apeloig
Ionization energies of triazines and tetrazines. Application of the Green's function method coupled with semiempirical molecular orbital calculations
Journal of Chemical Society. Perkin Transaction 2, №12, 1865-1873 (1991)

[26] **D. Danovich**
OVGF(SEMI): Molecular orbital package for outer valence Green's function calculations coupled with the MNDO, MNDOC, AM1, PM3 semiemperical approximation
QCPE Bulletin, **11**, №2, 31 (1991)

[27] **D. Danovich,** Y. Apeloig
Ionization energies of triazines and tetrazines. Application of the Green's function method coupled with semiempirical molecular orbital calculations
Journal of Chemical Society. Perkin Transaction 2, A collected volume to Commemorate the 150th Anniversary of the Royal Society of Chemistry, 97-105 (1992).

[28] V.K. Turchaninov, **D.K. Danovich**, A.F. Ermikov, M.A. Andriankov
Interpretaion of photoelectron spectra within the framework of the AM1 semiempirical method. 2. Pyridines
Bulletin of the Academy of Science of the USSR. Division of Chemical Science, **41**, 678-683 (1992)

[29] **D. Danovich**, Y. Apeloig, S. Shaik
A reliable and inexpensive method for calculating ionization potentials and electron affinities of radicals and molecules
Journal of Chemical Society. Perkin Transaction 2, №3, 321-330 (1993)

[30] 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 a curve-crossing analysis
Israel Journal of Chemisry, **33**, 387-402 (1993)

[31] U. Samuni, S. Kahana, R. Fraenkel, Y. Haas, **D. Danovich**, S. Shaik
The ICN-INC system: experiment and quantum chemical calculations
Chemical Physical Letters, **225**, 391-397 (1994)

[32] **D. Danovich**, J. Hrusak and S. Shaik
Ab initio calcuations for small iodo clusters. Good performance of relativistic effective core potentials
Chemical Phiysical Letters, **233**, 249-256 (1995)

[33] S. Shaik, A.C. Reddy, A. Ioffe, J.P. Dinnocenzo, **D. Danovich**, J.K. Cho
Reactivity paradigms: transition state sructure, mechanisms of barrier formation, and stereospecificity of nucleophilic substitutions on σ-cation radicals
Journal of the American Chemical Society, **117**, 3205-3222 (1995)

[34] 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 cation radicals
Journal of Chemical Socity. Perkin Transaction 2, 1525-1539 (1995)

[35] 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 energies
Journal of the American Chemical Society, **117**, 7760-7768 (1995)

[36] P.C.Hiberty, S. Humbel, **D. Danovich**, S. Shaik
What is physically wrong with the description of odd-electron bonding by Hartree-Fock theory? A simple nonempirical remedy
Journal of the American Chemical Society, **117**, 9003-9011 (1995)

[37] S. Shaik, **D. Danovich**, A. Fiedler, D. Schroder, H. Schwarz
Two-state reactivity in organometallic gas-phase ion chemistry
Helvetica Chimia Acta, **78**, 1393-1407 (1995)

[38] Y. Apeloig, **D. Danovich**
Ionization energies of linear and cyclc polysilanes. Application of the Green's function method coupled with semiempirical molecular orbital calculations
Organometallics, **15**, №1, 350-360 (1996)

[39] S. Shaik, A. Shurki, **D. Danovich**, P.C. Hiberty
Origins of the exalted B_{2u} frequency in the first excited state of benzene
Journal of the American Chemical Society, **118**, 666-671 (1996)

[40] G.N. Sastry, **D. Danovich**, S. Shaik
Towards the definition of the maximum allowable tightness of an electron transfer transition state in the reactions of anion radicals and alkyl halides
Angewante Chemie, International Edition English, **35**, 1098-1100 (1996)

[41] D. Lauvergnat, P.C. Hiberty, **D. Danovich**, S. Shaik
Comparison of the C-Cl and Si-Cl bonds. A Valence bond study
Journal of Physical Chemistry, **100**, 5715-5720 (1996)

[42] **D. Danovich**, S. Shaik
A Theoretical study of the role of spin-orbit coupling in the oxidative activation of H-H by FeO^+
Journal of the American Chemical Society, **119**, 1773-1786 (1997)

[43] **D. Danovich**
NDDO semiempirical approximations coupled with Green's function technique - a reliable approach for calculating ionization potentials
Journal of Molecular Structure (Theochem), Special Issue, **401**, 235-252 (1997)

[44] S. Shaik, A. Shurki, **D. Danovich**, P.C. Hiberty
A different story of benzene
Journal of Molecular Structure (Theochem), Special Issue, **398-399**, 157-167 (1997)

[45] J.N. Harvey, D. Schroeder, W. Kohn, H. Schwarz, **D. Danovich** and S. Shaik
Electron transfer reactivity in the bond activation of organic fluorides by calcium monocation
Journal of the Physical Chemistry, Part A, **273**, 164-170 (1997)

[46] 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
Journal of the American Chemical Society, **119**, 9237-9245 (1997)

[47] **D. Danovich**
Green's Function Method in Semiempirical Molecular Orbital Theory: Calculations of Ionization Potentials and Electron Affinities
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