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Chemistry
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Education:

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- M.S. (with honors) in Chemistry, minor in Physics, Jagiellonian University (Poland) 1976-1981
 - Ph.D. (with honors) in Chemistry, minor in Physics, Jagiellonian University (Poland) 1983-1988

Research Experience:

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- Assistant Professor, Jagiellonian University (Poland) 1988-2000
 - Postdoctoral Research Associate, University of Bonn (Germany) 1989-1991
 - Postdoctoral Research Associate, University at Buffalo NY, 1995-1997
 - Research Associate, University of Louisville KY, 2000-2001
 - Research Associate, University at Buffalo NY, 2001-2004
 - Computational Scientist, University at Buffalo NY, 2004-2009
 - Adjunct Assistant Professor, University at Buffalo NY, 2003-present
 - Research Assistant Professor, Southern Methodist University TX, 2010-present

Research Interest:

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- Investigations of chemical reactions using a reaction valley approach and a reaction path Hamiltonian.
 - Investigations of chemical structure and bonding using analysis of the electron density distribution.
 - Modeling of protein-drug interactions using docking and molecular dynamics simulations in explicit water solution.
 - Development of computational methods and their applications for biological systems, using massive parallel computing and utilizing a combined quantum mechanical - molecular mechanical (QM/MM) method.

- Development of theoretical models in electronic and vibrational spectroscopy

Teaching experience:

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- Undergraduate and graduate level courses: quantum chemistry, quantum mechanics, theoretical spectroscopy, group theory, thermodynamics, statistic physics, mathematics and computer programming; Jagiellonian University (Poland) 1981-2000.
 - Graduate level computer course: "Computer Modeling of Biological Systems"; University at Buffalo NY, 2007-2009.

Workshops organization and teaching:

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- Q-Chem Workshop in University California, Berkeley, CA, December 10-11, 2009.
 - Q-Chem Workshop in University of Illinois at Urbana-Champaign, Il, November 4-5, 2009, National Center for Supercomputing Applications, Urbana-Champaign, IL.
 - Q-Chem Workshop in Washington DC, August 15, 2009, NIH Bethesda campus, Washington, DC.
 - Q-Chem Workshop, May 19, 2009, Penn State University, State College, PA.
 - Q-Chem Workshop on Electronic Structure Calculations, March 19-20, 2009, Pittsburgh Supercomputing Center, Pittsburgh, PA.

Presentation at international conferences:

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- The 238th meeting of the American Chemical Society, Washington DC, USA, 2009, poster presenter.
 - The 9th Annual Conference on Structure-Based Drug Design, Cambridge Healthtech Institute, Boston, MA, USA, 2009, poster presenter.
 - The 7th International Conference on Bioinformatics and Bioengineering, Harvard Medical School, Boston, MA, USA, 2007.
 - The 2006 International Accelrys Conference, Baltimore, MD, USA, 2006, invited lecturer.
 - The 2006 International Conference on Bioinformatics and Computational Biology, Las Vegas, NV, USA, 2006, discussion presenter.
 - 230th meeting of the American Chemical Society, Washington DC, USA, 2005, invited lecturer.
 - Gordon Research Conference, New Hampshire, USA, 1996, poster presenter.
 - Computational Chemistry Conference, Lyon, France, 1995, invited lecturer.

Skills:

- Computational modeling using quantum chemical programs: Q-Chem, GAUSSIAN, CFOUR, MOLPRO, GAMESS, TURBOMOLE, JAGUAR, NWChem, COLUMBUS, MOLCAS, ADF, DALTON, MRD-CI, AMPAC/MOPAC, SPARTAN, GAUSSVIEW; and molecular mechanical programs: CHARMM, AMBER, BOSS.
- Quantum mechanical calculations: standard RHF and UHF, Complete Active Space SCF (CASSCF), Restricted Active Space SCF (RASSCF), Multireference CI method (MRCI), coupled cluster (CCSD(T)), MP2 method; calculations of potential energy surfaces, excited electronic states, spectroscopic parameters, electronic transition moments, spin-orbit couplings, reaction profiles, transition states, geometry optimization, molecular force fields, molecular oscillations.
- Density functional theory (DFT) and time dependent DFT (TDDFT) calculations.
- SFC calculations with the polarizable continuum model of solvent effects including the isotropic dielectrics, the anisotropic dielectrics, and the COSMO model.
- Molecular mechanical calculations: standard molecular mechanical Newton and Langevin dynamics in the gas phase and in water solution with periodic boundary conditions using the Particle Mesh Ewald method, Poisson-Boltzmann dynamics, molecular mechanical Monte Carlo simulations; calculations of solutions, proteins, DNA and inorganic polymers.
- Combined quantum mechanical - molecular mechanical (QM/MM) calculations: geometry optimization, molecular oscillations, transition states, and reaction profiles of an active site inside inorganic polymers and biopolymers like proteins and DNA in explicit water solution; binding drug molecules to active sites of proteins and DNA in explicit water solution, using molecular mechanical dynamics combined with high-level quantum mechanical calculations on a semiempirical, ab initio and DFT level of theory.
- Theoretical models of molecular electronic spectroscopy including vibronic transitions, Franck-Condon factors, Renner-Teller effect, Jahn-Teller effect, Herzberg-Teller effect, vibronic interactions in molecular dimers and trimers.
- Parallel and sequential computing using IBM SP Cluster, IBM RS/6000 Workstation, SGI Altix, SGI Origin, SGI Linux Cluster, SGI Workstation, Sun Enterprise Cluster, Sun Workstation, Convex, Cyber, DELL Linux Cluster, HP Linux Cluster.
- Programming in computational languages: FORTRAN (expert level), PASCAL (expert level), Delphi (expert level), HTML (expert level), Perl (expert level), Java (entry level).
- Scientific visualization using professional graphic software such as Adobe Illustrator, Adobe Photoshop, and Adobe Dreamweaver, supported by knowledge in photography at an expert level.

Publications:

- L. Muley, B. Baum, M. Smolinski, M. Freindorf, A. Heine, G. Klebe, D.G. Hangauer, 26 Enhancement of Hydrophobic Interactions and Hydrogen Bond Strength by Cooperativity: Synthesis, Modeling, and Molecular Dynamics Simulations of a Congeneric Series of Thrombin Inhibitors, *J. Med. Chem.*, accepted for publication.
- J. Kong, Z. Gan, E. Proynov, M. Freindorf, T. R. Furlani, Efficient computation of the dispersion interaction with density functional theory, *Phys. Rev. A*, 79, 042510 (2009).
- K.S. Shores, J.P. Charlebois, C.-T. Chiang, R.L. DeLeon, M. Freindorf, T.R. Furlani, J.F. Garvey, Reactions within p-Difluorobenzene/Methanol Heterocluster Ions: A Detailed Experimental and Theoretical Investigation. *J. Phys. Chem. A*, 113, 2268 (2009).
- C.-T. Chiang, K.S. Shores, M. Freindorf, T. Furlani, R.L. DeLeon, J.F. Garvey Size-Restricted 23 Proton Transfer within Toluene-Methanol Cluster Ions, *J. Phys. Chem. A*, 112, 11559 (2008).
- M. Freindorf, Y. Shao, J. Kong, T. R. Furlani, Combined QM/MM Calculations of Active-Site 22 Vibrations in Binding Process of P450cam to Putidaredoxin. *J. Inorg. Biochem.* 102, 427 (2008).
- M. Freindorf, Y. Shao, J. Kong, T. R. Furlani, Large-Scale QM/MM Calculations of Electronic 21 Excitations in Yellow Protein, Toward Petascale Level of Protein Calculations. Proceedings of the 7th International Conference on Bioinformatics and Bioengineering, Harvard Medical School, Boston, MA, USA, 614 (2007).
- C.-T. Chiang, M. Freindorf, T. F. Furlani, R.L. DeLeon, J.P. Richard, J.F. Garvey, Enhancement of a Lewis Acid-Base Interaction via Solvation: Ammonia Molecules and the Benzene Radical Cation, *J. Phys. Chem. A*. 111, 6068 (2007).
- M. Freindorf, Y. Shao, J. Kong, T. R. Furlani, Combined QM/MM Studies of Binding Effect of Cytochrome p450cam to Putidaredoxin, Proceedings of the 2006 International Conference on Bioinformatics and Computational Biology, Las Vegas, NV, USA, 391 (2006).
- C.-T. Chiang, M. Freindorf, T. F. Furlani, R.L. DeLeon, J.P. Richard, J.F. Garvey, Enhancement of a Lewis Acid-Base Interaction via Solvation: Ammonia Molecules and the Benzene Radical Cation, *J. Phys. Chem. A*. 111, 6068 (2007).
- M. Freindorf, Y. Shao, J. Kong, T. F. Furlani, A Combined Density Functional Theory and Molecular Mechanics (QM/MM) Study of FeCO Vibrations in Carbonmonoxy Myoglobin, (communication) *Chem. Phys. Letters*. 419, 563 (2006).
- D.N. Shin, M. Freindorf, T. R. Furlani, R.L. DeLeon, J.F. Garvey Nitrosamide, (H₂NNO), Formation within [(NO)_m(NH₃)_n]⁺ Clusters: Theory & Experiment, *I. J. Mass Spectrom.* 255–256, 28 (2006).

- M.Freindorf, Y.Shao, T.F.Furlani, J.Kong, Lennard-Jones parameters for combined 16 QM/MM method using B3LYP/6-31+G*/AMBER potential, *J.Comput.Chem.* 26, 1270 (2005).
- M.Freindorf, H.F.King, Ab initio MRCI potential energy surfaces of the lowest electronic states of C₂H molecule, in preparation.
- M.Freindorf, H.F.King, Ab initio MRCI study of core-core and core-valence electron correlation in electronic states of C₂ and molecule, in preparation.
- M.Freindorf, P.M.Kozlowski, A combined density functional theory and molecular 13 mechanics study of the relationship between the structure of coenzyme B12 and its binding to methylmalonyl-CoA mutase, *J.Am.Chem.Soc.* (communication), 126, 1928 (2004).
- M.Freindorf, P.M.Kozlowski, DFT study of the metal coordination center domain of Fe(II)- bleomycin, *J. Phys. Chem.A*, 105, 7267 (2001).
- J.Gao, M.Freindorf, Hybrid ab Initio QM/MM simulation of the N-methylacetamide in aqueous solution, *J.Phys.Chem.A.*, 101, 3182 (1997).
- J.Gao, N.Li, M.Freindorf, Hybrid QM/MM simulations yield the ground and excited state pK_a difference: phenol in aqueous solution, *J.Am.Chem.Soc.*, (communication), 118, 4912 (1996).
- M.Freindorf, J.Gao, Optimization of the Leonard-Jones parameters for a combined ab initio QM/MM potential using the 3-21G basis set, *J.Comput.Chem.*, 17, 386 (1996).
- M.Freindorf, C.Marian, B.A.Hess, Theoretical study of the electronic spectrum of the CoH molecule, *J.Chem.Phys*, 99, 1215 (1993).
- M.Freindorf, Vibronic couplings in excited state of hydrogen bond dimeric systems, *Acta Physica Polonica*, A78, 825 (1990).
- M.Freindorf, Herzberg-Teller interaction in benzene trimeric system, *Acta Physica Polonica*, A76, 547 (1989).
- M.Freindorf, Herzberg-Teller interaction in benzene dimeric systems. II. Application, *Acta Physica Polonica*, A73, 649 (1988).
- M.Freindorf, Herzberg-Teller interaction in benzene dimeric systems. I. Model, *Acta Physica Polonica*, A73, 635 (1988).
- M.Freindorf, Vibronic coupling in benzene derivatives. Trimeric systems, *Acta Physica Polonica*, A71, 985 (1987).
- M.Freindorf, Vibronic coupling in benzene derivatives. Dimeric systems, *Acta Physica Polonica*, A70, 461 (1986).
- M.Freindorf, Effect of frequency change on absorption spectra of molecular trimers, *Acta Physica Polonica*, A69, 679 (1986).