

## SELECTED PUBLICATIONS

Active-Space Symmetry-Adapted-Cluster Configuration-Interaction and Equation-of-Motion Coupled-Cluster Methods for High Accuracy Calculations of Potential Energy Surfaces of Radicals, Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, *J. Chem. Phys.* **2007**, 126, 164111-1 - 164111-28.

Extension of the Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian to Open-Shell Systems: A Benchmark Study, M. Wloch, J.R. Gour, and P. Piecuch, *J. Phys. Chem. A* **2007**, 111, 11359-11382.

Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei, M. Horoi, J.R. Gour, M. Wloch, M.D. Lodriguito, B.A. Brown, and P. Piecuch, *Phys. Rev. Lett.* **2007**, 98, 112501-1 - 112501-4.

A Comparative Assessment of the Perturbative and Renormalized Coupled Cluster Theories with a Non-iterative Treatment of Triple Excitations for Thermochemical Kinetics, Including a Study of Basis Set and Core Correlation Effects, J. Zheng, J.R. Gour, J.J. Lutz, M. Wloch, P. Piecuch, and D.G. Truhlar, *J. Chem. Phys.* **2008**, 128, 044108-1 - 044108-7.

Stereoelectronic Effects on Molecular Geometries and State-Energy Splittings of Ligated Monocopper Dioxxygen Complexes, C.J. Cramer, J.R. Gour, A. Kinal, M. Wloch, P. Piecuch, A.R.M. Shahi, and L. Gagliardi, *J. Phys. Chem. A* **2008**, 112, 3754-3767.

Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene, J.J. Lutz and P. Piecuch, *J. Chem. Phys.* **2008**, 128, 154116-1 - 154116-12.

A Comparison of Single-Reference Coupled-Cluster and Multi-Reference Configuration Interaction Methods for Representative Cuts of the  $H_2S(^1A)$  Potential Energy Surface, Y.Z. Song, A. Kinal, P.J.S.B. Caridade, A.J.C. Varandas, and P. Piecuch, *J. Mol. Struct.: THEOCHEM* **2008**, 859, 22-29.

## UNIVERSITY DISTINGUISHED PROFESSOR AND ADJUNCT PROFESSOR OF PHYSICS

(b. 1960)

M.Sc., 1983, Univ. of Wrocław;

Wrocław (Poland);

Ph.D., 1988, Univ. of Wrocław;

Postdoctoral Fellow, 1988-91, Univ. of Waterloo (Canada);

Adjunct, 1990-92, Univ. of Wrocław;

Postdoctoral Associate, 1992-93, Univ. of Arizona;

Visiting Assistant Professor, 1994-95, Univ. of Waterloo;

Visiting Assistant Professor, 1995-97, Univ. of Toronto;

Postdoctoral Associate, 1997-98, Univ. of Florida;

Adjunct Assistant Professor, 2000-2003, Univ. of Waterloo;

Alfred P. Sloan Research Fellow, 2002-2004;

Invited Fellow of JSPS and

Vis. Prof., Kyoto Univ. (Japan), 2005;

Vis. Prof., Univ. of Coimbra (Portugal), 2006;

The S.R. Palit Memorial Lecture, IACS, Kolkata (India), 2007;

Elected Member, Eur. Acad. of Arts, Sciences and Humanities, Paris, France.

Fellow of the American Physical Society

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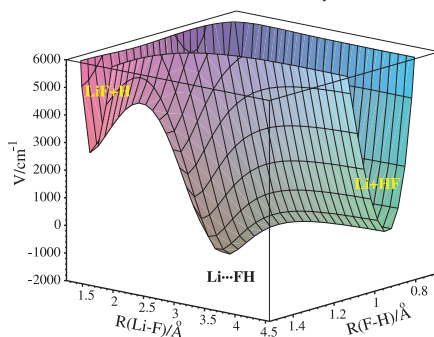
**M**y research focuses on (i) *ab initio* quantum theory of molecular electronic structure, nuclei, and other many-body systems, (ii) molecular properties and spectroscopy, (iii) reaction dynamics/mechanisms, and (iv) theory of intermolecular forces. One of the objectives of our research is to design and apply quantum-mechanical methods that enable precise determination of potential energy surfaces and property functions for both existing and hypothetical molecular systems in their ground and excited states. We are also interested in accurate quantum calculations for atomic nuclei and other many-body systems and calculations of intermolecular potentials and spectra for van der Waals complexes.

**Quantum theory of molecular electronic structure.** The key to understanding molecular electronic structure and dynamical behavior of molecules is an accurate assessment of the many-electron electron correlation effects. Our group focuses on new quantum-mechanical methods that include correlation, particularly on the coupled-cluster theory and its renormalized, extended, multi-reference, and response variants that allow us to study electronically excited states, bond breaking, electron-transfer processes, molecular properties in vibrationally and electronically excited states, and transition probability coefficients for various types of spectroscopy. Our primary interest is in high-accuracy methods that allow us to be predictive. We write computer codes for the standard and new coupled-cluster methods which are distributed world-wide through a popular electronic structure package, GAMESS.

**Many-body methods of quantum mechanics and nuclear physics.** Our new *ab initio* methods for many-electron systems can be applied to other many-fermion systems, including atomic nuclei. We have performed several highly successful *ab initio* coupled-cluster calculations for  $^4\text{He}$ ,  $^{16}\text{O}$ , and valence systems around  $^{16}\text{O}$  using modern nucleon-nucleon interactions. We have also carried out unprecedented coupled-cluster calculations for  $^{56}\text{Ni}$ . We are looking for the alternative approach

to accurate calculations for many-fermion systems with pair-wise interactions, including the use of two-body cluster expansions to represent the virtually exact many-fermion states.

**Molecular properties and spectroscopy.** We use linear-response coupled-cluster methods along with other *ab initio* approaches such as multi-reference configuration interaction method to calculate molecular multipole moments and (hyper)polarizabilities and the effect of nuclear motion on these properties. We use first-principles theories to obtain rovibrational and electronic spectra, including van der Waals precursors of photo-induced charge-transfer reactions.



**Reaction dynamics/mechanisms.** We have recently performed a series of successful computational studies of important organic chemistry reactions, including the Cope rearrangement of 1,5-hexadiene, cycloaddition of cyclopentyne to ethylene, thermal stereomutations of cyclopropane, and isomerization of bicyclo[1.1.0]butane to buta-1,3-diene. We have carried out unprecedented coupled-cluster calculations for  $\text{Cu}_2\text{O}_2$  systems relevant to oxygen activation by metalloenzymes and for photoisomerizations of acetylacetone. We have also studied the photo-induced charge-transfer ("harpooning") reactions between alkali and alkaline earth metal atoms and halides. In particular, we have combined *ab initio* and dynamical approaches to characterize quasi-bound states of van der Waals molecules that are precursors of these reactions.

**Theory of intermolecular forces.** Intermolecular potentials are a necessary ingredient for the determination of the structure, stability, and dynamics of weakly bound clusters and condensed phases. We are primarily interested in pair-wise non-additive interactions which are important when three or more atoms or molecules interact, although we also study interactions in dimers. We use state-of-the-art quantum chemistry to generate the necessary information about interacting species.