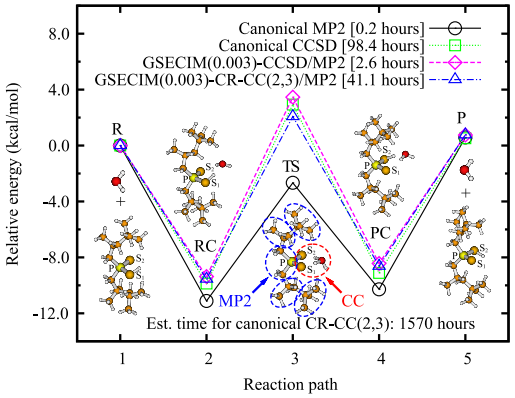
My research program focuses on (i) *ab initio* quantum theory of molecular electronic structure and other many-body systems, (ii) molecular properties, spectroscopy, and photochemistry, (iii) reaction mechanisms and dynamics, and (iv) theory of intermolecular forces. We design and apply quantum-mechanical methods that enable precise determination of potential energy surfaces and property functions for both existing and hypothetical molecular species in their ground and excited states. We are also interested in accurate quantum calculations for strongly correlated systems, weakly interacting molecular clusters, and atomic nuclei.

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 correlation effects. Our group focuses on the development and applications of new quantum-mechanical methods that include correlation, particularly on the coupled-cluster theory and



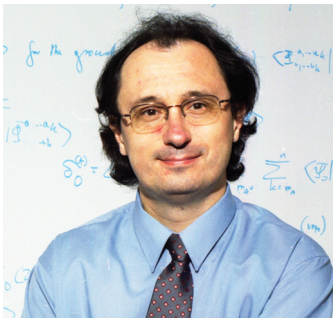
its renormalized, active-space, extended, multi-reference, and response variants that allow us to study bond breaking, electronically excited states, electron-transfer processes, molecular properties in vibrationally and electronically excited states, and transition probability coefficients for various types of spectroscopy. We examine ways of achieving high-level coupled-cluster or numerically exact energetics by combining deterministic computations with stochastic wave function sampling. We also develop approximate coupled-pair approaches for strongly correlated systems and local correlation coupled-cluster methods and their multi-level extensions that can be applied to high accuracy *ab initio* calculations for systems with hundreds of atoms. 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 and plugins to PSI4 available on GitHub. Some of our methods are also available in NW-Chem, Q-Chem, and MRCC packages.

Many-body methods of quantum mechanics and nuclear physics. We demonstrated that quantum-chemistry-inspired coupled-cluster methods can be applied to atomic nuclei. We performed several highly successful *ab initio* coupled-cluster calculations for ^{4}He, ^{16}O, and valence systems around ^{16}O using modern nucleon-nucleon interactions. We also carried out widely publicized coupled-cluster calculations for ^{56}Ni and its isotopes. We are looking for the alternative approaches to accurate calculations for many-fermion systems with pair-wise interactions, including the use of cluster expansions involving two-body correlation operators to represent nearly exact many-fermion states.

Molecular properties, spectroscopy, and photochemistry. We use linear-response coupled-cluster methods, along with other *ab initio* approaches, 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, electronic, and rovibronic spectra of molecules and weakly bound species. We have demonstrated that the lowest excited state of methylcobalamin should be interpreted as metal-to-ligand charge-transfer excitation and that azulene possesses the doubly excited state below the ionization threshold, which can drive multi-photon ionization experiments related to Rydberg fingerprint spectroscopy. We have provided definitive information about structural, electronic, and spectroscopic properties of several organic biradicals and small metal nanoparticles, including, for example, beryllium, magnesium, silver, and gold clusters.

Reaction mechanisms and dynamics. We performed successful computational studies for several 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 carried out unprecedented coupled-cluster calculations for CuO_2 and Cu_2O_2 systems, relevant to oxygen activation by metalloenzymes, for photoisomerizations of acetylacetone, for diffusion of atomic oxygen on the silicon surface, for proton-transfer reactions between the dithiophosphinic acids and water molecules, for aerobic oxidation of methanol on gold nanoparticles, and for the Co-C bond dissociation in methylcobalamin, relevant to catalytic properties of B_{12}. We also studied the photo-induced charge-transfer ("harpooning") reactions between alkali and alkaline earth metal atoms and halides. In particular, we combined *ab initio* and dynamical approaches to characterize quasi-bound states of van der Waals molecules that are precursors of these reactions.

Intermolecular interactions. Intermolecular potentials are a necessary ingredient for the determination of the structure, stability, and dynamics of weakly bound clusters and condensed phases. We are interested in many-body interactions, which are important when three or more atoms or molecules interact, and study interactions in dimers.



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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, 2000-03, Univ. of Waterloo;
Alfred P. Sloan Research Fellow, 2002-04;
Invited Fellow of JSPS and Vis. Prof., 2005, Kyoto Univ. (Japan);
Vis. Prof., Univ. of Coimbra (Portugal), 2006;
Palit Memorial Lecture, IACS, Kolkata, 2007;
Elected Member, Eur. Acad. of Arts, Sciences and Humanities, Paris, France, 2003;
Fellow of the American Physical Society, 2008;
Fellow of the American Association for the Advancement of Science, 2011;
Invited Prof., Inst. for Molecular Science, Okazaki (Japan), 2012-13;
Distinguished Fellow, Kosciuszko Foundation Collegium of Eminent Scientists, 2015;
Clark Way Harrison Distinguished Visiting Professor, Washington Univ. in St. Louis, 2016;
Fellow of the Royal Society of Chemistry, 2016;
Schaad Lectureship, Vanderbilt Univ., 2017;
Elected Member, International Academy of Quantum Molecular Science, 2018.

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Selected Publications

Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of Three-Particle–One-Hole and Four-Particle–Two-Hole Excitations, A.O. Ajala, J. Shen, and P. Piecuch, *J. Phys. Chem. A* **2017**, *121*, 3469.

Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC(P;Q) Methodology: Connected Quadruple Excitations, N.P. Bauman, J. Shen, and P. Piecuch, *Mol. Phys.* **2017**, *115*, 2860.

Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions, J.E. Deustua, J. Shen, and P. Piecuch, *Phys. Rev. Lett.* **2017**, *119*, 223003.

Application of the CC(P;Q) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer, I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, *J. Phys. Chem. A* **2018**, *122*, 1350.

Approaching Exact Quantum Chemistry by Cluster Analysis of Full Configuration Interaction Quantum Monte Carlo Wave Functions, J.E. Deustua, I. Magoulas, J. Shen, and P. Piecuch, *J. Chem. Phys.* **2018**, *149*, 151101.

Application of the Coupled-Cluster CC(P;Q) Approaches to the Magnesium Dimer, S.H. Yuwono, I. Magoulas, J. Shen, and P. Piecuch, *Mol. Phys.* **2019**, *117*, 1486.

Accurate Excited-State Energetics by a Combination of Monte Carlo Sampling and Equation-of-Motion Coupled-Cluster Computations, J.E. Deustua, S.H. Yuwono, J. Shen, and P. Piecuch, *J. Chem. Phys.* **2019**, *150*, 111101.