Chemistry and Physics Colloquium

Michigan Technological University

Thursday, March 27, 2008
4:00 - 5:00 pm
Room 139, Fisher Hall

Coupled-Cluster Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Atomic Nuclei

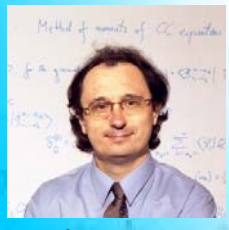
Piotr Piecuch

Department of Chemistry and Department of Physics and Astronomy
Michigan State University, East Lansing, Michigan 48824

ABSTRACT

The key to a successful description of many-electron and other many-fermion systems is an accurate assessment of particle correlations. One of the most efficient ways of describing many-electron correlations in molecules and many-nucleon correlations in atomic nuclei is offered by methods based on the coupled-cluster theory. This presentation will focus on the recently developed ideas in coupled-cluster theory that have resulted in the discovery of the renormalized coupled-cluster methods. It will be shown that renormalized coupled-cluster theories, which are based on the asymmetric energy expression that defines the method of moments of coupled-cluster equations, enable an accurate description of molecular potential energy surfaces involving bond breaking, reaction pathways in organic and bioinorganic chemistries, singlet-triplet gaps in magnetic systems, and excited electronic states with an ease of a black-box calculation that can be performed by experts as well as non-experts. It will also be shown that coupled-cluster theories can be extended to large molecular systems with hundreds of atoms, while retaining the high accuracies these methods offer for smaller molecular species, through suitably designed linear scaling algorithms. Finally, it will be demonstrated that the conventional and renormalized coupled-cluster methods, which have been developed in the context of electronic structure calculations, can find good use in nuclear physics, including the ground and excited states of the ^{4}He and ^{16}O nuclei, valence systems around ^{16}O, and heavier ^{55}Ni, ^{56}Ni, and ^{57}Ni nuclei, offering an alternative to the considerably more expensive shell-model calculations.

BIOGRAPHY



Professor Piecuch received his Ph.D. from the University of Wrocław, Poland in 1988. After postdoctoral and research faculty work at the Universities of Waterloo, Canada, Arizona, Toronto, Canada, and Florida, he joined the faculty at Michigan State University in 1998. He currently is a University Distinguished Professor in the Department of Chemistry and an Adjunct Professor in the Department of Physics and Astronomy at Michigan State University. He was also named a Visiting Professor at the University of Coimbra, Portugal, and Kyoto University, Japan. His research, described in about 160 publications, focuses on theoretical and computational chemistry and physics, particularly on the development and applications of many-body methods for accurate quantum calculations for molecular systems and atomic nuclei. He is an elected member of the European Academy of Sciences, Arts, and Humanities in Paris, France, and a recipient of a number awards, including the S.R. Palit Memorial Lecture at the Indian Association for the Cultivation of Science (Kolkata, India, 2007), the Invitation Fellowship of the Japan Society for the Promotion of Science (2005), the QSCP Promising Scientist Prize of Centre de Mécanique Ondulatoire Appliquée, France (2004), the Alfred P. Sloan Research Fellowship (2002-2004), the Wiley-International Journal of Quantum Chemistry Young Investigator Award (2000), and three awards from the Polish Chemical Society (1983, 1986, 1992).

MichiganTech