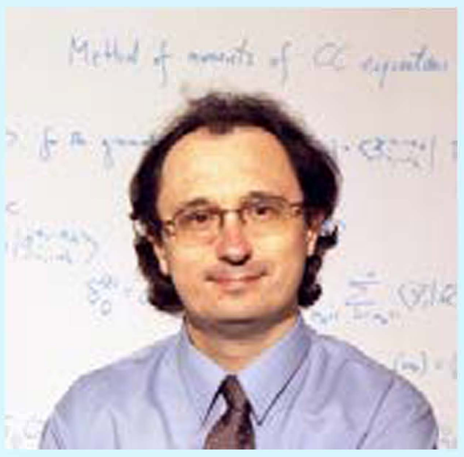
Approaching Exact Quantum Chemistry



Speaker: Prof. Piotr Piecuch

Invited by: Prof. Jian Liu

Michigan State University, East Lansing, Michigan, USA

Abstract

In this talk, we will examine a radically new way of obtaining accurate molecular electronic energies, equivalent to high-level coupled-cluster (CC) calculations, such as CCSDT or CCSDTQ, even when multireference correlation effects become significant. The key idea is a merger of the deterministic formalism, abbreviated as CC(*P*;*Q*), with the stochastic configuration interaction (CI) and CC Quantum Monte Carlo (QMC) approaches. We will also demonstrate that one can take the merger of the stochastic and deterministic ideas to the ultimate level and use it to extract the exact, full CI (FCI), energetics out of the early stages of FCIQMC propagations with the help of the relatively inexpensive polynomial steps similar to CCSD calculations, eliminating exponential complexity of conventional FCI Hamiltonian diagonalizations altogether. Extensions to excited electronic states by a combination of stochastic CIQMC and deterministic equation-of-motion CC computations and converging FCI energetics in strongly correlated systems (e.g., models of metal–insulator transitions), where the traditional CCSD, CCSDT, CCSDTQ, etc. hierarchy breaks down, will be discussed as well.

Honors and Awards

Professor Piecuch is a Fellow of the Royal Society of Chemistry, American Association for the Advancement of Science, and American Physical Society, an elected member of the International Academy of Quantum Molecular Science and European Academy of Sciences, Arts, and Humanities, and a Distinguished Fellow of the Kosciuszko Foundation Collegium of Eminent Scientists. Among his other honors are being named an Invited Fellow of the Japan Society for the Promotion of Science and Alfred P. Sloan Foundation Fellow.

Xingda: 11月15日 北大化学院 A204 报告厅 14:00-15:30