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Department of Chemistry

Moscowitz Memorial Lectureship

9:45 a.m. Thursday, April 14 • 331 Smith Hall

Professor

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Computational Quantum Chemistry: Two Extremes

Research interests include developing quantitative mathematical theories and computing algorithms to interpret and sometimes predict the properties and transformations of molecules, polymers and solids, and exploring new ways of numerically solving the fundamental equations of motion of chemistry

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Abstract

Two extreme examples of applications of computational quantum chemistry that are performed by the speaker's group are discussed. One aims at achieving essentially exact numerical solutions of the Schrodinger equations of small but general polyatomic molecules, combining powerful many-body methods, new basis functions that have explicit dependence on interelectronic distances, and computer algebra that can automate the derivation and computer implementation of exceedingly complex equations defining these methods. The other seeks to apply such high-accuracy computational methods to very large molecules such as polymers and molecular crystals by exploiting known characteristics of long-range chemical interactions and thereby accelerating the computational speed dramatically. A more fundamental question pertinent to the validity of statistical thermodynamics is addressed as to why energy per volume of a solid does not diverge and its thermodynamic limit exists.

The Moscowitz Memorial Lectureship in Chemistry was established by friends and colleagues of Professor Albert Moscowitz (1929-1996) to honor his many contributions to molecular spectroscopy. He was known for his research on the interpretation of optical rotation and circular dichroism spectra in terms of the structures of chiral molecules. In collaboration with colleagues in the medical sciences, he developed important applications of his methods to biomedical systems. Throughout his career, Moscowitz held numerous visiting professorships at other universities, and served on the editorial boards of the leading journals in chemical physics. His work was honored by election as Foreign Member of the Danish Royal Academy of Sciences and Letters, and as a Fellow of the American Physical Society.

Host: Professor Christopher Cramer
Refreshments will be served prior to the seminar.