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Department of Chemistry

Student Seminar Series

9:45 a.m. Tuesday, March 3, 2015 • 331 Smith Hall

Professor

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Electronic Structure Theory for Intermolecular Interactions

Website:
http://chem.berkeley.edu/faculty/head-gordon/index.php

Abstract

Progress in electronic structure calculations depends upon advances in the underlying methods used to accurately calculate intermolecular interactions at moderate cost, and also on the tools used for analyzing the results of calculations. After all, without analysis, electronic structure calculations are merely sophisticated numerical experiments. In this talk, I shall discuss recent progress on both fronts, and provide illustrative applications to intermolecular interactions ranging from physisorption through to conventional hydrogen bonds, and even stronger ionic hydrogen bonds and metal- ligand interactions. We shall look at disentangling dative (charge-transfer) interactions from polarization-dominated effects, and discuss some new theory that achieves improved separation of these physically distinct contributions to intermolecular interactions.

Professor Martin Head-Gordon is a professor of chemistry at the University of California, Berkeley, and Lawrence Berkeley National Laboratory working in the area of computational quantum chemistry. He is a member of the International Academy of Quantum Molecular Science, and one of the founders of Q-Chem Inc.

He earned his bachelor's degree in 1983 and master's degree in 1985 from Monash University in Australia, and doctorate in 1989 from Carnegie-Mellon University under the supervision of Professor John Pople. After three years of post-doctoral research at the AT&T Bell Laboratories, he joined the faculty of the University of California, Berkeley, and was promoted to full professor in 2000.

Professor Head-Gordon's research centers on the development of new electronic structure theory methods, and their implementation as efficient computer algorithms. Exciting progress has been made over the last few years in linear scaling methods for density functional theory, new approaches to describing the correlations between electrons in spatially localized terms, and new model chemistries for ground and excited states.

Professor Head-Gordon has received many prestigious awards, including a 1993 National Science Foundation Young Investigator Award, an Alfred P. Sloan Foundation Research Fellowship (1995-7), a David and Lucile Packard Fellowship (1995-2000), and the 1998 Medal of the International Academy of Quantum Molecular Science.

Host: Shaohong "Louis" Li