UCMERCED | CHEMISTRY & BIOCHEMISTRY

DATE 11/13/2026 | TIME 01:30pm | LOCATION COB1 267

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES

Density Functional Theory in Chemistry: Past, Present and Future

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Abstract:

Density functional theory only entered mainstream computational chemistry in the 1990s, almost 30 years after its formal foundations were made established, and about 20 years after the first pioneers began using it in chemistry. Why did it take so long, and what people and events were crucial in causing that change? This is the aspect of DFT's past that I will discuss. Regarding present-day DFT, I will describe some recent developments from my group aimed at improving hybrid density functionals. First, seeking the broadest accuracy that is possible for hybrid density functionals, I will summarize our new Carefully Optimized and Appropriately Constrained Hybrid (COACH). Second, I will discuss new work that aims to provide hybrid DFT calculations with error estimates, and show that transferable and useful error estimates can be obtained using statistical theory. These error estimates can also be applied to energy differences, and even differences of energy differences, to reflect the extent of error cancellation. Finally, I will attempt to offer a few thoughts on the future of DFT in chemistry.

About the Speaker:

Martin Head-Gordon completed B.Sc. (Hons) (1983) and M. Sc. (thesis) (1985) degrees at Monash University in Melbourne Australia, before coming to America to obtain his Ph. D. (1989) in theoretical chemistry at Carnegie-Mellon University, working with the late Sir John Pople on molecular orbital theory and algorithms. From 1989-1992 Head-Gordon was a postdoctoral fellow at AT&T Bell Laboratories, working with John Tully. He explored gas-surface energy exchange, and developed new models for non-adiabatic energy flow. Since 1992 Head-Gordon has been on the faculty of the Chemistry Department at the University of California Berkeley, where he holds the Kenneth S. Pitzer Distinguished Professorship (since 2012). He also holds an additional appointment as a Senior Faculty Scientist in the Chemical Sciences Division of Lawrence Berkeley National Laboratory.

Head-Gordon's research is primarily in molecular electronic structure theory. He is known for development of linear scaling quantum chemistry methods, for development of new density functionals, for advances in energy decomposition analysis, and for work on catalysis modeling. He is one of the driving forces behind the Q-Chem quantum chemistry program. Head-Gordon is a Fellow of the Royal Society (2019), a member of the National Academy of Sciences (2015), an American Chemical Society Fellow (2012), a member of the American Academy of Arts and Sciences (2011), and member of the International Academy of Quantum Molecular Sciences (2006). He is an Associate Editor of Molecular Physics and is the President of the World Association of Theoretical and Computational Chemists (WATOC).

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