Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Thursday, November 22nd, 2018 – 13:00 p.m.
CFEL Seminar room IV (Bldg. 99)

Prof. Fred Manby

Centre for Computational Chemistry, University of Bristol, UK

An introduction to coupled-cluster theory, and recent developments in quantum embedding

Coupled-cluster theory has become a key tool in quantum chemistry, providing gold-standard accuracy for ground- and excited-state energetics, and other properties. In this talk I will give a pedagogical introduction to how coupled-cluster theory works, from the perspectives of both the coupled-cluster wavefunction and the underlying diagrammatic many-body theory. One challenge for the application of coupled-cluster theory in chemistry is its computational expense. I will describe efforts in our group and elsewhere to use multiscale embedding theories to capture the benefits of coupled-cluster accuracy at greatly reduced computational cost; in particular I will show that combinations of coupled-cluster and density functional theory provide an attractive framework for accurate modelling of chemical reactivity.

Host: Angel Rubio

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