From one to one million atoms: fast and accurate quantum simulation methods

A talk by Johannes Dieterich
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DATE / TIME: Monday, 15th of January 2017, 04:00 p.m.

LOCATION: TU Wien, Seminarraum 138C (Freihaus, Turm B/yellow, 9. OG)

This lecture will introduce different quantum mechanics-based simulation methods for the simulation of small to big systems up to a million atoms.

In particular, local multi-reference singles and doubles configuration interaction theory (MRSDCI), embedding methods, and orbital-free density functional theory (OFDFT) will be discussed. Accuracy and efficiency of these methods will be highlighted, alongside recent implementation strategies, and their use for sustainable energy research.