Max-Planck-Institut für Struktur und Dynamik der Materie

Max Planck Institute for the Structure and Dynamics of Matter

Monday, July 4th 2016 – 14:00 CFEL Seminar room III (Blgd. 99)

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Coupled Cluster Theory for Strong Correlations

Coupled cluster theory is the dominant method in wave function-based calculations in systems of small to moderate size. It provides exceptionally accurate predictions for a wide array of energetics and properties. Moreover, it is size extensive, meaning that it can fruitfully be applied to condensed systems, provided only that one has computational resources sufficient for the task. Unfortunately, coupled cluster theory often breaks down in the presence of strong correlations, such as those responsible for superconductivity or various magnetically-ordered states. In this talk I discuss several modifications of the underlying theory which permits us to describe these kinds of technologically relevant problems while remaining within the powerful framework provided by the coupled cluster family of methods.



