TECHNISCHE UNIVERSITÄT WIEN

INSTITUT FÜR FESTKÖRPERPHYSIK
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EINLADUNG zum IFP-SEMINAR

Towards chemical accuracy in metals using coupled-cluster theories

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Host: Andreas Grüneis

Termin: Mittwoch, 20. März 2024, 16:00 Uhr

Ort: TU Wien, Freihausgebäude
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Vor dem Vortrag gibt es ab 15:30 Kaffee und Kekse

Abstract:

Coupled-cluster theories can be used to compute ab initio electronic correlation energies of real materials with systematically improvable accuracy. Nonetheless, the widely used coupled-cluster singles and doubles plus perturbative triples [CCSD(T)] method is only applicable to insulating materials. In the case of zero-gap materials, the truncation of the underlying many-body perturbation expansion leads to an infrared catastrophe. In order to tackle this challenge, we present a novel perturbative triples formalism, denoted as (cT), which yields convergent correlation energies in metallic systems. Additionally, the computed correlation energies for the three-dimensional uniform electron gas at metallic densities are in good agreement with, the highly accurate, quantum Monte Carlo results. At the same time, the newly proposed method retains all desirable properties of CCSD(T), such as its accuracy for insulating systems, as well as its low computational cost ($O(N^7)$), compared to the full inclusion of the triples in CCSDT ($O(N^8)$). Ultimately, this paves the way for ab initio calculations of real metals with chemical accuracy.