



EINLADUNG zum IFP-SEMINAR

Calculating defects in solids using equation-of-motion coupled-cluster

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Host: Christoph Eisenmenger-Sittner
Termin: Mittwoch, 18. Jänner 2023, 16:00 Uhr
Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

In this seminar we will talk about using coupled-cluster methods in order to calculate ground and excited states of defects in periodic systems using plane waves as a basis set. Defects are important both as a theoretical benchmark system and for practical applications in industry. We will present some calculations of optical excitation energies for color centers and comment some future directions in this area.

Special care will be taken in order to make the presentation intelligible to researchers with a physics background. Therefore, the talk will be held in a pedagogical manner striving to be self-contained.