MAX-PLANCK-INSTITUT
FÜR DYNAMIK KOMPLEXER
TECHNISCHER SYSTEME
MAGDEBURG

CSC Seminar

SPEAKER

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TITLE

Reliable and efficient methods for computing DFT properties and derivatives

ABSTRACT

Density-functional theory (DFT) is one of the most widely employed methods in quantum chemistry and solid-state physics to model the electronic structure. For the case of density functional theory on periodic systems, discretised using plane-wave basis sets, I will present an overview of our recently proposed methods to efficiently and reliably compute the DFT response properties. I will further discuss our algorithmic differentiation framework to compute DFT derivatives implemented in the Julia-based Density-Functional Toolkit (https://dftk.org). This framework in particular enables the computation of arbitrary derivatives of DFT ground state quantities versus input parameters, a first for plane-wave DFT. Amongst others this covers derivatives, which are relevant for inverse materials design, i.e. the systematic discovery of novel materials by optimising structural or design parameters in a way the materials exhibit desired properties.

Wednesday, August 28, 2024 at 3:00 pm
seminar room Prigogine