Stuttgarter Physikalisches ONLINE Kolloquium

Max-Planck-Institut für Festkörperforschung
Max-Planck-Institut für Intelligente Systeme
Fachbereich Physik, Universität Stuttgart

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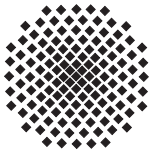

Login data will be announced by e-mail and on the colloquium webpage: www.physik.uni-stuttgart.de/aktuelles/kolloquium

Dienstag, 7. Juli 2020 **16.15 Uhr**

Stuttgarter Max-Planck-Institute, Heisenbergstraße 1, 70569 Stuttgart-Büsnau

Predicting materials properties from first-principles with generalized functionals for energy and spectra

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Abstract

In order to understand, predict, or design the properties of materials from first-principles we need to make sure that our electronic-structure methods are accurate enough for the problem at hand, and that they can capture the complexity of the materials or the processes studied. The strength of density-functional theory has come from being most often an accurate, inexpensive, and ultimately simple approach to ground-state energies, leading to the capability of studying not only complex systems, but complex processes - from transport coefficients to spectroscopic signatures. I'll start illustrating the variety and complexity of the materials properties that can be predicted these days with electronic-structure simulations, and then discuss some of the simplest but most damaging failures, showcasing how generalized Hubbard functionals (for energies) or Koopmans functionals (for spectra) can achieve very inexpensively the predictive accuracy sought for in complex, realistic systems.