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Stuttgarter Physikalisches Kolloquium

Max-Planck-Institut für Festkörperforschung
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Hybrid

Login data will be announced by e-mail and on the colloquium webpage.

Dienstag, 24. Juni 2025	16.15 Uhr	Lecture Hall 2D5

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Numerical Tools to Predict Electron Dynamics in Correlated Quantum Solids: The Example of NiO

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Abstract

Understanding the dynamics of electrons in materials is essential for interpreting the behaviour of systems as diverse as solar cells, batteries, and catalysts. However, predicting electron dynamics in correlated quantum materials poses significant theoretical challenges. Dynamical properties often arise from competing interactions, including local correlations, multiplet effects, charge transfer, covalency, and band formation. Despite the possibility for low-lying excitations to decay through multiple channels, long-lived excitations or quasi-particles with well-defined energy-momentum dispersions can still exist. Theoretical predictions of such dynamics must cover time scales many orders of magnitude longer than the inverse of the dominant energy scales, making numerical material-realistic simulations particularly demanding.

We present a theoretical approach that combines nonlinear response theory with diagrammatic expansions, real-frequency solvers based on renormalisation group methods, and truncated configuration interaction techniques to meet this challenge. Our method is suited for describing pump-probe spectroscopies ranging from THz to X-ray frequencies, capturing the electronic dynamics of materials across a wide energy range. As an application, we demonstrate the method on NiO, achieving quantitative predictions of optically pumped and probed photoelectron spectra and their long-lived coherent dynamics.