



SFB1242

Nichtgleichgewichtsdynamik kondensierter
Materie in der Zeitdomäne

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ESSEN

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Computational Quantum Materials: Protocols & Examples

Prof. Dr. Cesare Franchini

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In this talk, we shall discuss the application of single-particle and pseudo/quasi-particle approaches for the calculation of the properties of complex materials from a first principles perspective. Beside reviewing the fundamental theories we describe the technical procedures to obtain quantitative predictions without adjustable parameters using self-consistent hybrid functionals (scPBE0), GW, the Bethe-Salpeter equation (BSE), and DFT+U with interaction parameters U/J derived from the constrained random phase approximation. Specific topics include: band gaps and band structure, convergence protocols in GW (comparison between the conventional approach based on an incremental variation of a specific set of parameters and the basis-set extrapolation scheme), optical properties using the BSE and model-BSE methods, magnetic exchange interactions within spin and pseudospin effective theories. Most of the examples will focus on (spin-orbit coupled) transition metal oxides, where the entanglement of orbital, spin and lattice interactions gives rise to collective effects which are difficult to model and understand, but are of key importance for disclosing the nature of new quantum phases of matter and for practical functionalizations.

Für diese Zeit steht eine Kinderbetreuung nach vorheriger Anmeldung zur Verfügung.

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