FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

# PhD position at the Friedrich-Alexander-University Erlangen

## *"Cellular dynamical mean-field theory for Charge-Transfer Transition Metal Oxides"*

DFT DMFT cDMFT

The two natural quantum mechanical starting points to approach solids in theoretical physics are **i) the limit of almost free electrons and ii) the limit of almost free atoms**. Usually the former is the first step taken in introductory courses as it connects seamlessly to basic problems encountered in basic quantum mechanics courses. By assuming that effects of the interactions between electrons can be approximated with an external (mean-field) potential we remain with single particle Schroedinger equations for periodic potentials and arrive at Bloch-wave eigenfunctions and their bandstructure. Indeed, until today the most successful method for the simulation of electronic structure in real materials - Density functional theory (DFT) - is based on such mapping to the "best possible effective single particle problem".

The opposite limit is, in contrast, a focus on the isolated building blocks of the lattice, i.e. the atoms. Instead of mapping the two-particle Coulomb scattering to an external potential, hybridization and interaction of the surrounding lattice are treated approximately beyond the free standing atom. Exact diagonalization of finite size many-body Hamiltonians for atoms/ions (or small coordination complexes) with partially filled shells in non-spherical potentials, i.e. crystal- (ligand-) field theory, is the most basic approximation of this kind. While such localized crystal and ligand field approximations usually work extremely well for predictions inside Mott- (Charge transfer-) insulating phases, they are insufficient to capture coherent quasiparticle excitations around the Fermi level of a metal. **Dynamical Mean-Field Theory** (DMFT) allows to bridge this gap and cross the insulator to metal phase transition from the localized (or Mott-) state to the Fermi liquid metal. The "dynamical" nature of DMFT captures the metallic state as quantum super- position of different atomic configurations and yields the exact solution for the single particle self energy of the Hubbard model in the limit of infinite dimensions (or coordination number) at any correlation strength.

The PhD project is aimed at a **real-space cluster extensions of dynamical mean-field theory**. Besides studies on paradigmatic models like the 2D Hubbard model on different lattice geometries or the Emery model for cuprate superconductors, material realistic models for transition metal oxides (TMO) of charge transfer (CT) and negative charge transfer (NCT) character will be focus.

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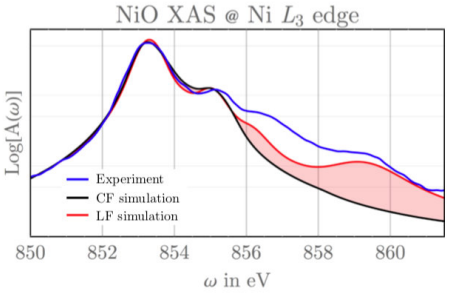


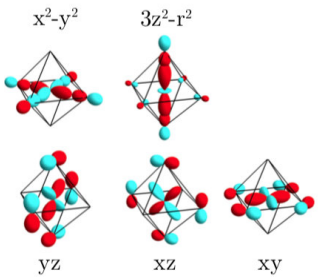


*Advanced many-body methods connected to state-of-the-art measurement techniques allows for a crucial theory-experiment interface.*

*Here, core-level absorption spectroscopy shows the importance of oxygen degrees of freedom for ground state properties in the so called charge transfer material NiO*

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The group of Philipp Hansmann at the FAU Erlangen-Nuernberg offers the candidate contact to an international network of leading groups in the field of quantum many-body physics and correlated electron materials. Among others, ongoing collaborations include groups at the CCQ at the Flatiron institute (NYC), and at the TU Wien. *The position is financed for 36 months.*

Ideally the candidate has a strong background in *quantum mechanics, solid state physics, and statistical physics*. Knowledge of 2nd quantization as well as basic coding experience (e.g. Python, C++) is advantageous.

Please send your **coverletter, CV *(including master certification with grades)*** to *philipp.hansmann@fau.de*