CSSI Element: SI2-SSE: Collaborative Research: Software Framework for Strongly Correlated Materials: from DFT to DMFT

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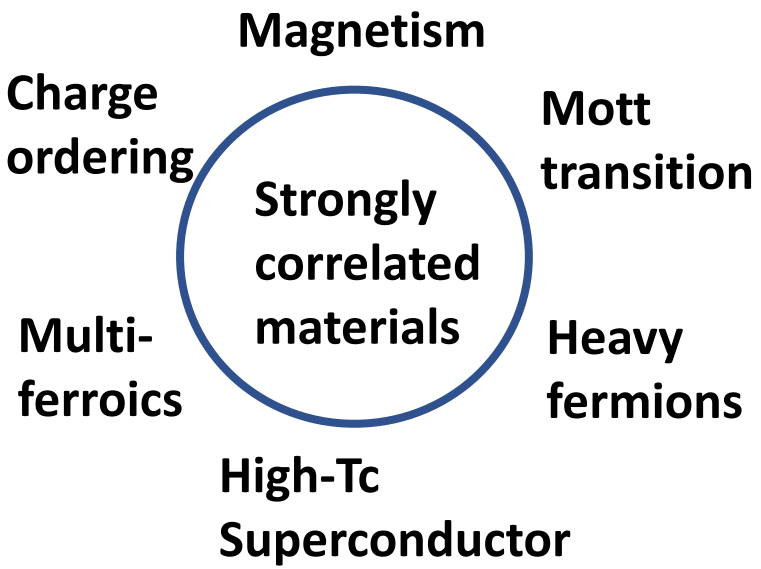
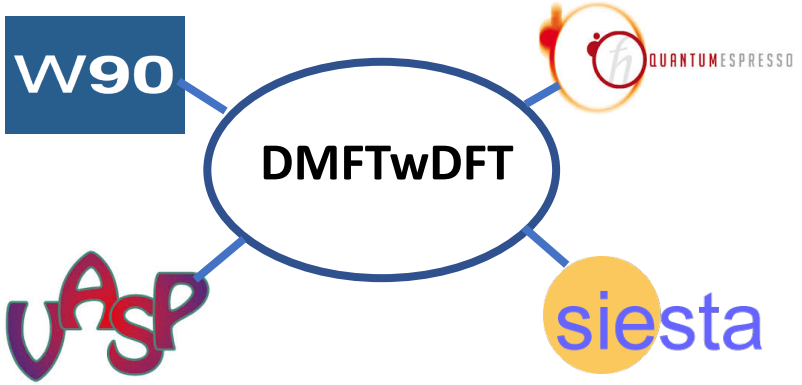
Motivation



- **Challenge:** Understanding novel material properties via strong correlation from first-principles

DMFTwDFT package

- **Interfaced to various electronic structure packages**



- We developed an open-source and Python-interface package (DMFTwDFT) combining DMFT with various DFT codes for strongly correlated materials

Features of the code

- Library mode: an efficient link of our package to an arbitrary DFT codes.
- Post-processing tools: band structures, density of states, and total energies of materials.
- Parallelization using MPI

Future directions

- Implementation of atomic forces, phonons, and the Fermi surface calculations in our package
- Application of the code to the study of rare-earth materials and oxides with oxygen vacancies and defects.