

solid_dmft: gray-boxing DFT+DMFT materials simulations with TRIQS

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Summary

Strongly correlated systems are a class of materials whose electronic structure is heavily influenced by the effect of electron-electron interactions. In these systems, an effective single-particle description may not capture the many-body effects accurately. Although density functional theory (DFT) plus dynamical mean-field theory (DMFT) has proven successful in describing strongly correlated electron systems for over two decades, it has only been very recently that ready-to-use software packages began to become available, with most scientific research carried out by self-written codes developed and used in research groups. Given the complexity of the method, there is also the question of whether users should implement the formalism themselves for each problem or whether ready-to-use black-box software, as is the case with many DFT software packages, is beneficial to the community.

The goal of solid_dmft is to find a middle ground, i.e., a *gray-box* tool as a ready-to-use implementation. This means that while the code contains all the functionality needed for many standard DMFT calculations, it is highly modular, based on open-source and community-developed software, and therefore can be easily adapted to specific applications and needs. Hence, this project is targeted towards researchers aiming to apply DMFT methods on top of DFT simulations to describe the physics of strongly correlated electron systems. While our approach allows one to fully perform these computations using standardized input flags without need for coding, the final user can easily extend the functionalities by modifying the corresponding modules in the code.

The package is MPI-parallelized and written in Python 3, utilizing the publicly available TRIQS software library ([Parcollet et al., 2015](#)) and the applications based on TRIQS, such as different solvers or DFT interfaces. The philosophy of the package is to increase reproducibility of DFT+DMFT calculations, provide clearer convergence metrics, and allow one to run calculations for a large variety of systems without adapting the code manually, i.e., on a level similar to widely available DFT simulation packages.

Design Principles

solid_dmft uses the state-of-the-art implementations provided by the TRIQS ecosystem. This allows the user to easily run ab-initio calculations for strongly correlated materials, as well as implement and test new features of TRIQS and benchmark new TRIQS solvers against existing ones. solid_dmft either manages the DFT run itself in charge self-consistency or simply uses the DFT output for one-shot calculations, then creates the downfolded Hamiltonian, solves the resulting Hubbard-like Hamiltonian via DMFT, postprocesses the data to calculate physical observables, and allows feeding back the corrected charge via charge self-consistency. The full DFT+DMFT cycle is presented in [Figure 1](#).

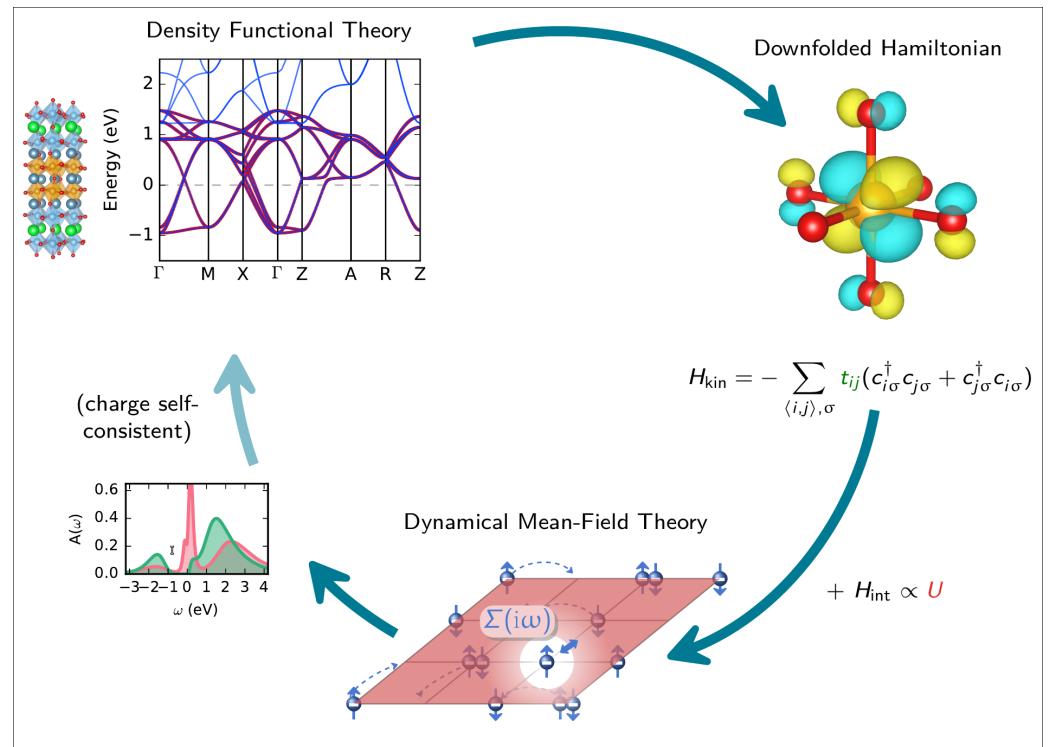


Figure 1: Fully charge self-consistent DFT+DMFT cycle. Starting from a DFT calculation (top left), a downfolded Hamiltonian and projector functions are created via optimized projections on a local basis set (top right). By adding a specified interaction Hamiltonian H_{int} , a full interacting electron problem is created, to be solved via the DMFT equations in TRIQS (bottom). After convergence in DMFT is reached, physical observables are calculated (bottom left). For fully charge self-consistent calculations, the DFT cycle is restarted with a DMFT-corrected charge density.

43 The code is designed to run on the output of a DFT calculation or a tight-binding model,
44 which provide the low-energy (downfolded) description of a periodic system. This DFT output
45 is converted into a standardized HDF5 archive by TRIQS/DFTTools (Aichhorn et al., 2016) to
46 be used by solid_dmft so that all DFT codes compatible with TRIQS/DFTTools are supported.
47 The input for the DMFT calculation can be provided either as a Hamiltonian in reciprocal
48 \mathbf{k} -space in a localized basis set or in terms of the overlap between the localized basis set and
49 the Kohn-Sham wavefunctions (so-called projector functions) and their respective eigenvalues.

50 The code follows the same modular philosophy as the TRIQS software package and relies
51 on TRIQS functionalities to perform basic operations on Green functions. Each part of the
52 simulation is split into separate stand-alone functions to limit statefulness to a minimum and
53 allows easily extending the functionalities. The modularity of the program also allows users to
54 run, for example, the DMFT loop via a call of a single pure function with well-defined input
55 and output, i.e., without running solid_dmft as a monolithic code. An abstracted solver
56 class implements the various impurity solvers available in TRIQS. solid_dmft allows one to
57 seamlessly switch between impurity solvers with the change of a simple input flag and by
58 adjusting the solver parameters. Fully charge self-consistent interfaces are implemented for
59 Quantum ESPRESSO (Giannozzi et al., 2009) and the Vienna ab-initio simulation package
60 (VASP) (Kresse & Furthmüller, 1996; Kresse & Hafner, 1993). solid_dmft also allows users
61 to perform inhomogeneous DMFT calculations, i.e., the treatment of multiple correlated and
62 uncorrelated shells (impurity problems). Postprocessing scripts are available to perform analytic
63 continuation of imaginary Green functions or self-energies, and to calculate spectral functions.

64 As of now, solid_dmft has been successfully used in various peer-reviewed research studies
65 (Beck et al., 2022; Hampel et al., 2019, 2020, 2021; Merkel & Ederer, 2021; Zhang et

al., 2022). We provide releases matching those of the TRIQS library, as well as up-to-date documentation with automatic API documentation and tutorials. Examples and benchmark calculations can be found in the tutorials section of the documentation. Furthermore, we utilize a continuous-integration workflow on GitHub to test every pull request and commit.

Statement of need

As of now, only few ready-to-use DFT+DMFT codes are available, all of them released rather recently. Most of these codes adopt a black-box approach, where the complexity of the DMFT part is abstracted away from the final user (as in EDMFT (Haule et al., 2010), Amulet (Poteryaev & others, n.d.) or the DMFT implementation in Abinit (Romero et al., 2020)) and therefore reduces the number of free parameters to tune. However, this approach may limit the flexibility of the implementation. `solid_dmft` is designed as a more modular, and open source implementation, similar to other software packages like DFTwDMFT (Singh et al., 2021) and DCORE (Shinaoka et al., 2021), and acts as a flagship program connecting the TRIQS functionality. The benefits of this approach are twofold: on the one hand, developers of the TRIQS ecosystem are able to benchmark their applications in a well-tested framework. On the other hand, users can benefit from a standardized input-output structure compatible with the TRIQS framework, fundamentally increasing robustness and reproducibility. `solid_dmft` is developed in the spirit of a community code and supports external contributions that advance the capabilities of the software.

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