




# 1 solid\_dmft: gray-boxing ab initio DFT+DMFT utilizing 2 TRIQS

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## Software

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## 8 Summary

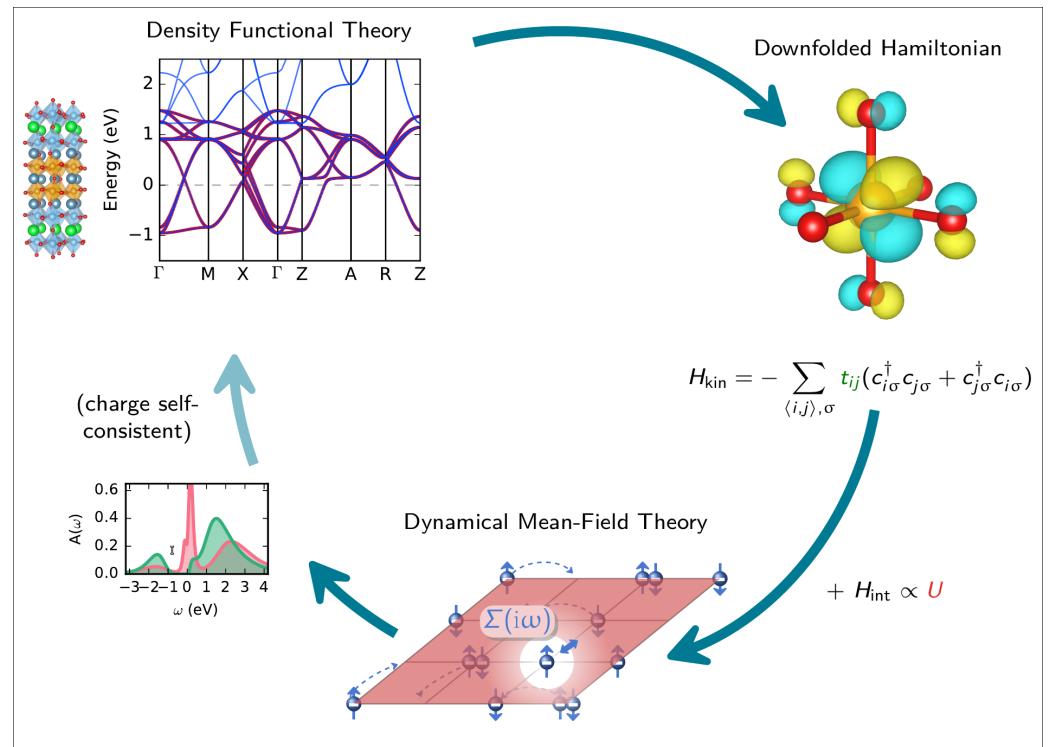
9 Strongly correlated systems are a class of materials whose electronic structure is heavily  
10 influenced by the effect of electron-electron interactions. In these systems, the attempt of  
11 an effective single-particle description often fails, and one has to explicitly take into account  
12 coulombic and exchange effects. Although density functional theory (DFT) plus dynamical  
13 mean-field theory (DMFT) has proven successful in describing strongly correlated electron  
14 systems for over two decades, it has only been very recently that ready-to-use software packages  
15 began to become available, with most scientific research carried out by self-written codes  
16 developed and used in research groups. Given the complexity of the method, there is also the  
17 question of whether users should implement the formalism themselves for each problem or  
18 whether ready-to-use black-box software, as is the case with many DFT software packages, is  
19 beneficial to the community.

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

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

## 34 Design Principles

35 The idea is to provide the full functionality of a full DFT+DMFT calculation by merging the  
36 state-of-the-art implementations provided by the TRIQS library and its applications. This  
37 allows to easily run ab-initio calculations for strongly correlated materials, as well as implement  
38 and test new features of TRIQS or benchmark new solvers against existing ones. solid\_dmft  
39 manages the calls of the necessary routines to run the DFT calculations, create the downfolded  
40 Hamiltonian, solve the resulting Hubbard-like Hamiltonian via DMFT, postprocess the data to  
41 calculate physically meaningful observables, and allow for charge-corrected feedback via charge  
42 self-consistency. The full DFT+DMFT cycle is presented in [Figure 1](#).



**Figure 1:** Full CSC 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  $H_{\text{int}}$ , a full interacting electron problem is created, to be solved via the DMFT equations (bottom) in TRIQS. After convergence in DMFT is reached, physical observables are calculated (bottom left). For fully CSC calculations a charge density correction is added to DFT and the cycle is restarted.

The code is designed to run on top of a DFT calculation or model system providing a low-energy (downfolded) description of the periodic solid system. The DFT calculations can be performed with any code that is compatible with TRIQS/DFTTools (Aichhorn et al., 2016). The input for the DMFT calculation can be either provided directly as a Hamiltonian in reciprocal  $\mathbf{k}$ -space in a localized basis set, or in terms of the overlap between the localized basis set and the Kohn-Sham wavefunctions (so-called projector functions), and their respective eigenvalues. The DFT output is converted by TRIQS/DFTTools into an HDF archive in a standardized structure to be read or written into by solid\_dmft.

The code is designed to be modular in the same philosophy as the TRIQS software package, relying on TRIQS functionalities to perform basic operations. Therefore, we split each part of the simulation into separate stand-alone functions, to limit statefulness to a minimum and allow for an easy extension to include new features. The modularity of the program also allows to run, for example, the DMFT loop only via a call of a single function with well-defined input and output, i.e., without running solid\_dmft as a monolithic code. This ensures that the code can be used in other projects. An abstracted solver class implements the various impurity solvers available in TRIQS. Even though different solvers operate differently, solid\_dmft allows to seamlessly switch impurity solvers, with a simple input flag and adjusting the solver parameters. A fully charge self-consistent (CSC) interface is implemented for Quantum ESPRESSO and the Vienna ab-initio simulation package (VASP). solid\_dmft allows also to perform inhomogeneous DMFT calculations, i.e., the treatment of multiple correlated and uncorrelated shells (impurity problems) while converging the full lattice self-energy. After self-consistency is reached, either via full CSC or just within the DMFT cycle, postprocessing scripts are available to perform analytic continuation of imaginary Green's functions, and to calculate spectral functions.

As of now, `solid_dmft` has been successfully used in various peer-reviewed research studies (Beck & Georges, 2022; Hampel et al., 2019, 2020, 2021; Merkel & Ederer, 2021; Zhang et al., 2022), and provides stable releases matching the releases of the TRIQS library. We provide a full documentation including several tutorials and a reference manual. Examples and benchmark calculations can be found in the tutorials section of the documentation. Furthermore, we utilize an extensive CI workflow on GitHub to test every pull request and commit.

## Statement of need

As mentioned, the number of ready-to-use DFT+DMFT codes is small, and all codes have been developed rather recently. Crucially, 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 while such a strategy can reduce the numbers of free parameters to tune, it also inevitably hinders the flexibility of the approach. Other software packages like DFTwDMFT (Singh et al., 2021) and DCORE (Shinaoka et al., 2021) follow a very similar strategy as `solid_dmft`. Most notably, `solid_dmft` provides a flagship implementation of the TRIQS functionality to perform DFT+DMFT calculation and is easily extended. The benefits of this approach are twofold: on the one hand, developers of TRIQS applications 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 rest of the TRIQS ecosystem, allowing for easy reproducibility of results.

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.

`solid_dmft` is developed in the spirit of a community code and supports external contributions that advance the capabilities of the program.

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