Consistent self-consistent merging of GW and EDMFT : Tiers of approximations

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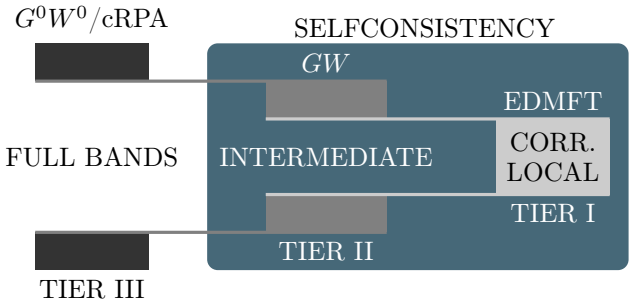

Multiple tiers in a ab-initio materials investigation

We address systems with strongly correlated orbitals by systematically treating the least relevant degrees of freedom in the system with an appropriate approximation, thereby constructing the parameters for the next tier, the higher relevance model. This is repeated from the Local Density Approximation (LDA) density functional calculation for the full space of bands as the lowest tier all the way to a Continuous Time Quantum Monte Carlo (CTQMC)[1] simulation of an effective impurity problem, subject to retardation effects on the effective bare propagator and interaction through non-local and off-low-energy correlation and polarization effects. In the simplest case this is equivalent to GW+EDMFT,[2,3] but puts it into a consistent, double-counting free, extensible ab-initio framework. We discuss the effect of self-consistency in this approach.
As an application we discuss the presumably prototypical strongly correlated perovskite $SrVO_3$ for which the conventional interpretation of the 'Hubbard' peaks will need to be reconsidered.

1. Gull, E, Millis, A, Lichtenstein, A, Rubtsov, A, Troyer, M, Werner, P, *Continuous-time Monte Carlo methods for quantum impurity models*, Rev. Mod. Phys. 83, 349, 2011

2. Biermann, S, Aryasetiawan, F, Georges, A, *First-Principles Approach to the Electronic Structure of Strongly Correlated Systems : Combining the GW Approximation and Dynamical Mean-Field Theory*, Phys. Rev. Let. 90, 86402, 2003

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