An implementation of LDA+DMFT within the PAW framework: Application to SrVO3. BERNARD AMADON, CEA Bruyeres le Chatel, DPTA, France, FRANK LECHERMANN, University of Hamburg, Germany, ANTOINE GEORGES, Ecole Polytechnique, CNRS, France — The combination of LDA and DMFT has been used in the past ten years to understand properties of strongly correlated systems. Different interfaces have been used such as Linear Muffin Tin Orbitals and Maximally Localized Wannier Functions. Such schemes are however restricted to simple systems because the construction of wannier functions is demanding or because another simplification is used (such as the atomic sphere approximation). We present a new implementation of LDA+DMFT, which keeps the precision of the Wannier implementation, but which is lighter. It relies on the projection of Kohn-Sham states over localized orbitals to define the correlated subsystem. We have implemented this method within the Projector Augmented Wave framework. This thus opens the way to electronic structure calculations within LDA+DMFT for more complex structures. We present an application to SrVO3. The results are compared to calculations done on the Wannier basis and we discuss the features of the total spectral function.

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