Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Fully self-consistent LDA+DMFT calculations in the projector augmented wave (PAW) framework BERNARD AMADON, MARC TORRENT, CEA-DAM DIF — The combination of Density Functional Theory (DFT) in the Local Density Approximation (LDA) and Dynamical Mean Field Theory (DMFT) has been used in the past years to understand properties of strongly correlated electron systems. Recently, implementations have emerged based on state-of-the art density functional theory codes. We present here a implementation of LDA+DMFT, using projected local orbitals, which includes full self-consistency on the electronic density, within the Projector Augmented Wave (PAW) framework. This thus opens the way to accurate calculations including relaxation with the simplicity of a plane wave code and the all-electron precision. We benchmark this implementation on correlated metals and insulators.

Bernard Amadon
CEA-DAM DIF

Date submitted: 25 Nov 2009 Electronic form version 1.4