Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Free energy from stationary implementation of the DFT+EDMFT functional TURAN BIROL, KRISTJAN HAULE, Rutgers University — The workhorse of first principles calculations on crystalline solids is the Density Functional Theory at the level of Local Density Approximation (LDA). Despite its various successes, LDA is prone to an overbinding problem, which introduces an error in optimized lattice constants and other structural parameters. Various Generalized Gradient Approximations are introduced to correct for this problem, but they often fail to systematically correct it, in particular in correlated electron materials. We developed a stationary and functional derivable Embedded Dynamical Mean Field Theory combined with the DFT (EDMFT+DFT) to calculate the free energy and to optimize the structural parameters in correlated electron compounds. In our stationary formalism, the first order error in the density leads to a much smaller, second order error in the free energy. We consider the correlated metal $SrVO_3$, Mott insulating FeO, elemental Ce, and iron chalcogenide FeSe as examples to show that EDMFT predicts the lattice constants with high accuracy.

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Date submitted: 06 Nov 2015 Electronic form version 1.4