Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Implementation of parameter-free LDA+DMFT and GW+DMFT for diatomic molecules using exact double-counting correction JUHO LEE, KRISTJAN HAULE, Rutgers Univ — Dynamical Mean Field Theory (DMFT) in combination with Local Density Approximation (LDA) is widely used in solids to predict properties of correlated systems. Here one of the simplest strongly correlated systems, the hydrogen molecule H_2, is used as a testbed to develop a parameter-free LDA+DMFT framework. We propose a method to calculate the exact intersection of LDA and DMFT that leads to highly accurate subtraction of the doubly counted correlation in both methods. The total energy accuracy of LDA+DMFT in its single site version is around 0.3%, provided that a good projector to the correlated subspace and the exact double-counting treatment are used. In addition to LDA+DMFT, we also implement combined GW and DMFT for diatomic molecules. The total energy accuracy of GW+DMFT is as remarkable as that of LDA+DMFT is, while the excitation spectrum is predicted in even better agreement with the exact theory.

Juho Lee
Rutgers Univ

Date submitted: 14 Nov 2014 Electronic form version 1.4