Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Including short length scale correlations in quantum chemistry methods K. BHASKARAN-NAIR, Louisiana State University, K. KOWALSKI, Pacific Northwest National Laboratory, J. MORENO, W. SHELTON, M. JARRELL, Louisiana State University — Many aspects of computational chemistry and computational material science require accuracies that can only be obtained by a small class of highly accurate computational methods that appropriately account for instantaneous interactions between electrons in molecules or in materials. To aid in addressing the sign problem associated with DMFT based methods we use accurate quantum chemistry methods to treat short length scale correlations within DMFT type formulations and its cluster extensions. The local Green function is obtained from truncated variants of Configuration Interaction and Coupled Cluster methods, which efficiently describe the electron correlation effects. This work is supported by the National Science Foundation award NSF EPS-1003897 with additional support from the Louisiana Board of Regents.

Juana Moreno
Louisiana State University

Date submitted: 15 Nov 2013 Electronic form version 1.4