Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Correlation matrix renormalization approximation for total energy calculations of correlated electron systems[1] Y.X. YAO, C. LIU, J. LIU, Ames Laboratory and Iowa State University, W.C. LU, Jilin University and Qingdao University, C.Z. WANG, K.M. HO, Ames Laboratory and Iowa State University — The recently introduced correlation matrix renormalization approximation (CMRA) was further developed by adopting a completely factorizable form for the renormalization z-factors, which assumes the validity of the Wick's theorem with respect to Gutzwiller wave function. This approximation (CMR-II) shows better dissociation behavior than the original one (CMR-I) based on the straightforward generalization of the Gutzwiller approximation to two-body interactions. We further improved the performance of CMRA by redefining the z-factors as a function of f(z) in CMR-II, which we call CMR-III. We obtained an analytical expression of f(z) by enforcing the equality in energy functional between CMR-III and full configuration interaction for the benchmark minimal basis H2. We show that CMR-III yields quite good binding energies and dissociation behaviors for various hydrogen clusters with converged basis set. Finally, we apply CMR-III to hydrogen crystal phases and compare the results with quantum Monte Carlo.

[1]Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. DOE by Iowa State University under Contract No. DE-AC02-07CH11358.

Yongxin Yao
Ames Laboratory and Iowa State University

Date submitted: 15 Nov 2012 Electronic form version 1.4