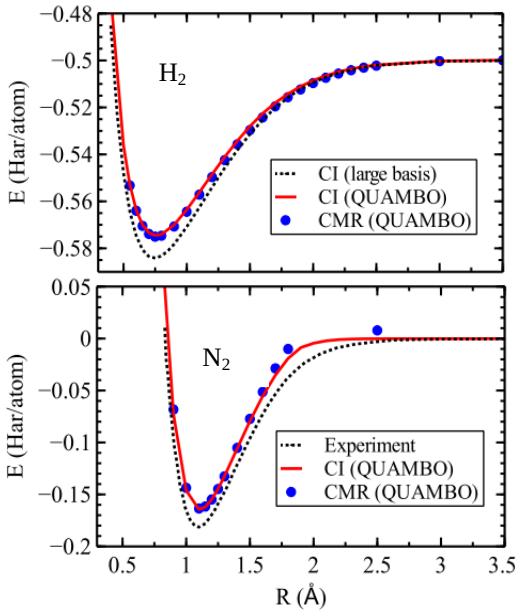
CORRELATION MATRIX RENORMALIZATION METHOD FOR TOTAL-ENERGY CALCULATIONS OF CORRELATED ELECTRON SYSTEMS

Yong-Xin Yao[(a)], Chen Liu[(a)], Jun Liu[(a)], Cai-Zhuang Wang[(a)], Kai-Ming Ho[(a)]

[(a)] Ames Laboratory of U.S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

ABSTRACT

We developed an *ab initio* correlation matrix renormalization (CMR) method[1,2], which a) renormalizes the two-electron correlation matrix by assuming the validity of Wick's theorem; b) modifies the commonly-used Gutzwiller orbital renormalization factor according to the exact analytical solution of the minimal basis hydrogen molecule; and c) adds a two-electron correction term due to the sum-rule violation. We show that the CMR method produces binding energy curves in close agreement with full configuration interaction (FCI) calculations in a series of tested molecules using minimal basis set orbitals. The calculations using the optimized quasi-atomic minimal basis set orbitals [3] are also shown to be quite close to the large basis FCI or experimental results.



Binding energy curves (circles) of H_2 and N_2 molecules calculated by the correlation matrix renormalization method, compared with the full CI results (solid lines) using the optimized quasi-atomic minimal basis set orbitals. The exact (dotted lines, full CI with large basis set or experimental) results are also shown for reference.

1. Yao, Y. X., J. Liu, C. Z. Wang, and K. M. Ho. 2014. "Correlation Matrix Renormalization Approximation for Total-Energy Calculations of Correlated Electron Systems." Physical Review B 89 (4): 045131. doi:10.1103/PhysRevB.89.045131.
2. Yao, Y. X., J. Liu, C. Liu, W. C. Lu, C. Z. Wang, and K. M. Ho. 2015. "Efficient and Accurate Treatment of Electron Correlations with Correlation Matrix Renormalization Theory." Scientific Reports 5 (August): 13478. doi:10.1038/srep13478.
3. Lu, W. C., C. Z. Wang, T. L. Chan, K. Ruedenberg, and K. M. Ho. 2004. "Representation of Electronic Structures in Crystals in Terms of Highly Localized Quasiatomic Minimal Basis Orbitals." Physical Review B 70 (4). doi:10.1103/PhysRevB.70.041101.