

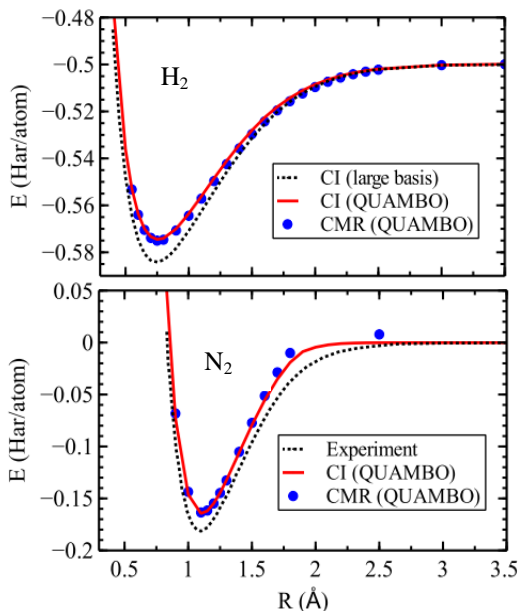
# CORRELATION MATRIX RENORMALIZATION METHOD FOR TOTAL-ENERGY CALCULATIONS OF CORRELATED ELECTRON SYSTEMS

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## 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<sub>2</sub> and N<sub>2</sub> 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.

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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.
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