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Correlation matrix renormalization method for correlated electron systems and application to crystalline phases of atomic hydrogen

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We recently developed a correlation matrix renormalization (CMR) method to calculate the electronic structures and total energies of correlated electron systems [1,2]. The CMR method goes beyond the conventional Gutzwiller approximation and incorporates Coulomb interactions between two localized electrons on different atomic sites, yet the computational speed of the CMR can be reduced to a level similar to Hartree-Fock calculations. Benchmark calculations on a set of molecules show the CMR method describes well the binding energies and bond-breaking behavior of these molecules in comparison with accurate quantum chemistry calculations [3]. Application of the CMR method to the studies of energy verses volume behavior for several crystalline phases of atomic hydrogen also produces results in good agreement with available results from quantum Monte Carlo calculations.

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References

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