EXTENSION OF CORRELATION MATRIX RENORMALIZATION METHOD TO TRANSITION METAL DIMERS AND MAGNETIC CALCULATIONS

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ABSTRACT

The correlation matrix renormalization (CMR) method [1,2,3] is benchmarked by calculating the binding energy curve of Cr_2 dimer, which is a well-established testbed for the accurate treatment of electron correlation effects. The crucial basis-set convergence effect will be discussed to achieve reasonable agreement with the experimental result. To go beyond some intrinsic limitations of CMR, we propose a more rigorous method without resorting to the commonly used inter-site decoupling approximation. The new method features ideal parallel efficiency. We demonstrate its accuracy and efficiency by evaluating the potential energy curves of nonmagnetic Cr_2 dimer and magnetic O_2 dimer.

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