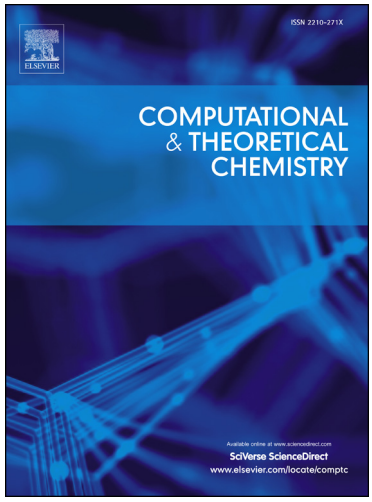

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Performance of the completely renormalized equation-of-motion coupled-cluster method in calculations of excited-state potential cuts of water

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Abstract

The left-eigenstate completely renormalized (CR) coupled-cluster (CC) and equation-of-motion CC (EOMCC) approaches with singles, doubles, and non-iterative triples, abbreviated as CR-CC(2,3) and CR-EOMCC(2,3), respectively, are used to generate cuts of the low-lying potential energy surfaces (PESs) corresponding to the dissociation of the water molecule into the OH and H fragments. The performance of the CR-CC(2,3) and CR-EOMCC(2,3) methods is evaluated by comparing the results with those obtained in the full configuration interaction and multi-reference CC (MRCC) calculations reported earlier by Li and Paldus [J. Chem. Phys. 133 (2010) 024102]. It is shown that the single-reference, black-box CR-CC(2,3) and CR-EOMCC(2,3) methods produce PESs that are competitive with those obtained with the expert high-level MRCC approaches.

Keywords: Coupled-cluster theory, Equation-of-motion coupled-cluster methods, Completely renormalized equation-of-motion coupled-cluster approaches, Excited electronic states, Potential energy surfaces, Water dissociation

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