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Ab-Initio-Based Approach to Study Complete Metalloproteins: Divide and Conquer Geometry Optimization of Nitric-Oxide Reductase
YUTAO YUE, TEEPANIS CHACHIYO, JORGE H. RODRIGUEZ, Department of Physics, Purdue University, West Lafayette, IN 47907-2036 — The direct application of ab-initio methods (Hartree-Fock or density functional theory) to study complete biomolecules has been impossible due to the huge computational cost of fully quantum mechanical calculations. As an initial step towards overcoming this problem, we implemented an ab-initio-based method to predict geometric structures of large metalloproteins using the principle of "divide and conquer." The method has been applied to small test systems showing satisfactory agreement with all-atom ab initio calculations. We have successfully applied the divide and conquer approach to partially optimize the geometry of a ligand-enzyme system, namely NO binding to nitric-oxide reductases (NOR, P450nor). NOR is a metalloenzyme that catalyzes the reduction of NO to N_2O. To compare our results with all atom calculations we studied a biochemically relevant subsystem (375 atoms) of the ligand-enzyme complex. The deviation between the divide and conquer geometry and the all atom partial geometry optimization is minor, on order of $10^{-}1$ Å for bond lengths. The computational cost of the method is moderately expensive making its application to large (bio) molecules plausible. Supported by NSF CAREER Award CHE-0349189 (JHR).

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