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Superoxide dismutase activity of Cu-bound prion protein MIROSLAV HODAK, NC State University, WENCHANG LU, JERRY BERNHOLC, NC State University and ORNL — Misfolding of the prion protein, PrP, has been linked to a group of neurodegenerative diseases, including the mad cow disease in cattle and the Creutzfeldt-Jakob disease in humans. The normal function of PrP is still unknown, but it was found that the PrP can efficiently bind Cu(II) ions. Early experiments suggested that Cu-PrP complex possesses significant superoxide dismutase (SOD) activity, but later experiments failed to confirm it and at present this issue remains unresolved. Using a recently developed hybrid DFT/DFT method, which combines Kohn-Sham DFT for the solute and its first solvation shells with orbital-free DFT for the remainder of the solvent, we have investigated SOD activity of PrP. The PrP is capable of incorporating Cu(II) ions in several binding modes and our calculations find that each mode has a different SOD activity. The highest activity found is comparable to those of well-known SOD proteins, suggesting that the conflicting experimental results may be due to different bindings of Cu(II) in those experiments.

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