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The role of metallic ions in nano-bio hybrid catalysts from *ab initio* first principles[1] SUSHANT BEHERA, PRITAM DEB, Department of Physics, Tezpur University, Tezpur-784028, India — We employ high-accuracy linear-scaling density functional theory calculations [*PRB* **84**, 165131, 2011] with a near-complete basis set and a minimal parameter implicit solvent model, within the self-consistent calculation, on silver ion assimilated on bacteriorhodopsin (bR) at specific binding sites. The geometry optimization indicates the formation of stable active sites at the interface of nano-bio hybrid and density of states reflects the metallic behavior of the active sites. Detailed kinetics of the catalytic reaction is revealed using *ab initio* electronic structure calculations. We observed that the metal ion incorporated active sites are more efficient in electrolytic splitting of water than pristine sites due to their less value of Gibbs free energy for hydrogen evolution reaction and strong synergistic effect [*PCCP* **18**(33), 23220, 2016]. The volcano plot analysis and free energy diagram are considered to understan hydrogen evolution efficiency. Moreover, the essential role of metallic ion on catalytic efficiency is elucidated.

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