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Modeling of hydrogen evolution reaction on the surface of $GaInP_2$[1] WOON IH CHOI, BRANDON WOOD, ERIC SCHWEGLER, TADASHI OGITSU, LLNL, QUANTUM SIMULATION GROUP TEAM — $GaInP_2$ is promising candidate material for hydrogen production using sunlight. It reduces solvated proton into hydrogen molecule using light-induced excited electrons in the photoelectrochemical cell. However, it is challenging to model hydrogen evolution reaction (HER) using first-principles molecular dynamics. Instead, we use Anderson-Newns model and generalized solvent coordinate in Marcus-Hush theory to describe adiabatic free energy surface of HER. Model parameters are fitted from the DFT calculations. We model Volmer-Heyrovsky reaction path on the surfaces of CuPt phase of $GaInP_2$. We also discuss effects of surface oxide and catalyst atoms that exist on top of bare surfaces in experimental circumstances.

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