Theoretical Insights to Glycerol Adsorption on β- Niooh Surface

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Density functional theory +U calculations have investigated the interaction of glycerol with a β-NiOOH (001) surface to determine the abilities of this surface to electrocatalytically accelerate the glycerol oxidation reaction. In addition, the adsorption energies of glycerol on the β-NiOOH (001) surface were calculated by selecting the different positions of glycerol on this surface to determine how glycerol preferentially adsorbs. The results emphasized the importance of a hydroxyl group on a glycerol molecule to the β-NiOOH (001) surface and how the glycerol orientation causes to find the most stable system.