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Shape-tunable electronic properties of H-passivated Si nanowires

ABRAHAM HMIEL, YONGQIANG XUE, University at Albany-SUNY — In this work we explore the structure, energetics and electronic properties of hydrogen-passivated silicon nanowires (SiNWs) with different surface structures and growth directions using first principles density functional theory. We first demonstrated that [112]-oriented Si nanowires (SiNWs) show a indirect-to-direct band gap transition induced solely by varying the cross sectional aspect ratio for both monohydride and trihydride passivation, which is explained by the different confinement effects on the conduction band state at Gamma point by the two facets. By analyzing the free energy of formation, we found that direct band gap [112] SiNWs are thermodynamically possible to form at experimentally relevant conditions. We next study water monomer adsorption on [112] and [110] SiNWs. We present results on adsorption geometry/energy and adsorption-induced electronic effects and investigate their shape/diameter dependence.

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