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Effect of hydrogen passivation on the structure and energetics of silicon nanowires ABRAHAM AHMIEL, YONGQIANG XUE, SUNY Albany — In this work we explore systematically the structure, energetics and electronic properties of silicon nanowires (SiNWs) with different surface structures and growth directions, and the trend of such property variation with increasing nanowire diameters using first principles density functional theory with both local atomic basis and plane waves. Both passivated and unpassivated systems were studied. The unpassivated (100) and (111) wires are found to be metallic with the unpaired electrons on the surface of these wires acting as conducting channels. Hydrogen passivation of these surfaces introduces a direct band gap by confining the electrons to localized bonds. The nature of the electronic states is examined through local density of states and electron density distributions. The relative stability of SiNWs with different growth directions and surface structures are evaluated from the free energy of formation.

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