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Surface Passivation and Orientation Dependence in the Electronic Properties of Silicon Nanowires KEENAN ZHUO, Georgia Institute of Technology, Atlanta, Georgia, USA, MEI-YIN CHOU, Insitute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan and Georgia Institute of Technology, Atlanta, Georgia, USA — Different surface passivation configurations for silicon nanowires (SiNWs) have previously been studied for expanding their technological applications. Of note, methyl (CH_3) passivated SiNWs have enhanced ambient stability, while electronegative atoms/groups such as halogens are useful in band gap engineering and chemical post-processing. Thus far though, fundamental mechanisms for how such passivations alter the electronic properties of SiNWs have not been rigorously scrutinized. In this work, we address this issue through first-principles calculations on CH_3, fluorine (F) and hydrogen (H) passivated [110] and [111] SiNWs. In comparison to H passivation, we explain how CH_3 and F passivations cause significant band gap reductions in [110] SiNWs, through strain and quantum confinement respectively. Furthermore, we discuss how structural differences in [111] SiNWs mitigate these effects, thereby giving the electronic properties of [111] SiNWs greater stability against various surface passivations than those of [110] SiNWs.

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