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Electronic properties of fluorine passivated silicon nanowires: density functional calculations KEENAN ZHUO, MEI-YIN CHOU, Georgia institute of technology — Arrays of silicon nanowire(SiNWs) have recently gained attention as a promising new photovoltaic technology. Previous studies show that halogen passivated SiNWs have good chemical stability and also form a critical pathway towards organic group functionalization. Yet, surface halogens are known to alter the SiNW electronic structure, most notably by reducing the band gap. We explore the fundamental physics behind this effect through first principles calculations on hydrogen and fluorine passivated (110) SiNWs. Electronic structure analysis reveals that the highly electronegative fluorine passivation modifies the quantum confinement potential and induces changes in the energy level ordering. Furthermore, we show how a modified cylindrical potential well model can demonstrate a link between this quantum confinement modification and the shift in energy levels responsible for the band gap reduction.

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