Tuning the Electronic Band-Gap of 3C-Silicon Carbide Nanowires by Passivating with Different Chemical Species

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Silicon carbide (SiC) is well known to be a wide band gap semiconductor material with different stable polytypes such as 3C, 2H, 4H and 6H [1]. The corresponding nanowires (SiCNWs) are good candidates for applications in nanoelectromechanical sensors [2], nanocatalytic elements [3], and nano-optical circuits [4] capable of operating in harsh environments and high power applications. The larger band gap also results in a higher breakdown field, which is a useful property in electronic applications under extreme environments.

SiCNWs have quite different electronic structures in comparison with their bulk crystalline counterpart due to quantum confinement. While bulk SiC is a poor optoelectronic material due to its indirect band gap, SiCNWs can have a direct band gap and optical activity and then the effect of quantum confinement on the SiC NW band structure has been extensively explored [5]. However, the use of surface modification for band structure engineering has received less attention despite its potential importance. SiC surface modification is frequently used in microelectronic device processes. Some computational studies have shown the importance of oxygen-coverage in SiCNW [6], but the effects of surface chemical modifications on the SiCNW electronic structure have not been systematically investigated.

In this work, by using density-functional calculations, we investigate the effect of SiCNW surface covering with H, F, and OH, respectively, on the electronic properties of [111]-oriented 3C-SiCNWs, with different widths (see Figure 1). The results indicate that the surface chemistry and the diameter have important effects on the band structure and the density of states; allowing for the manipulation of the electronic states of 3C-SiC NWs (Figure 3).

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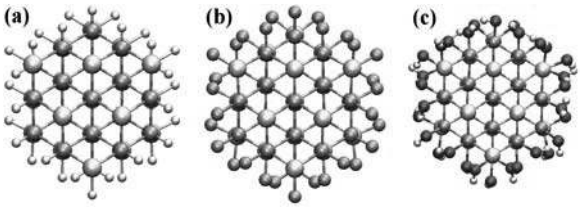

Fig. 1 Optimized (a) H-, (b) F-, (c) OH-passivated [111] 3C-SiC nanowires.

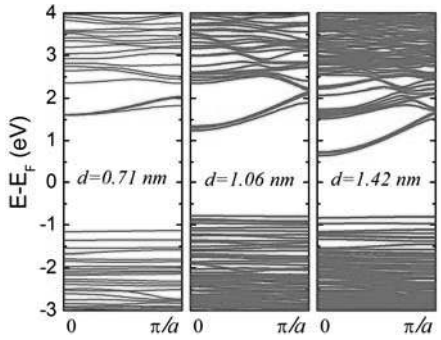

Fig. 2 Electronic band structure of OH-passivated SiCNWs with diameters of 0.71 nm, 1.06 nm and 1.42 nm.

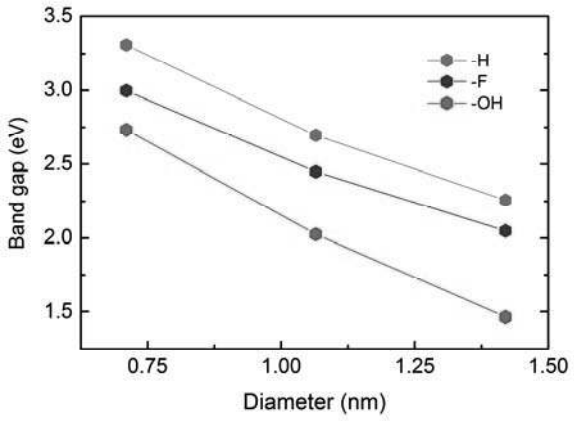

Fig. 3 Band gaps of H-, F- and OH-passivated [111] SiCNWs as a function of the diameter.

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