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Structural and Electronic Properties of Silicon Carbide Nanowires[1] SANGUO SHEN, M. YU, C. LEAHY, C.S. JAYANTHI, S.Y. WU, University of Louisville — We have studied the structural and electronic properties of SiC nanowires (NWs) of different diameters (1 nm < d < 7nm) and shapes (*e.g.*, hexagonal, round, and rhombohedral cross-sections) for wires oriented along <001>, <011>, <111> (cut from the 3C-bulk), and <0001> directions (cut from 2H-, 4H-, or 6H- bulk). A supercell is set-up for each of the above orientations. We relaxed the structures using the state-of-the-art semi-empirical molecular dynamics scheme as described in Ref. [1]. The main results of our findings are: (i) Among the different shapes investigated, NWs with hexagonal morphology are the most stable structures, (ii) Among the hexagonal NWs, those cut from 2H-SiC bulk structures were found to be the most stable ones in the diameter range investigated. They exhibit very weak surface relaxations, and were found to exhibit semiconductor characteristics, (iii) On the other hand, NWs cut from 3C-, 4H-, and 6H- bulk structures exhibit strong facet reconstructions and were found to have metallic characteristics. These results are in agreement with DFT-based ab-initio calculations for small diameter NWs up to 3 nms. [1] Leahy *et al.* Phys. Rev. B74, 155408 (2006).

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