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Tuning the electronic band-gap of fluorinated 3C-silicon carbide nanowires[1] ÁLVARO MIRANDA DURÁN, ALEJANDRO TREJO BAÑOS, ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430 México D.F., México, LUIS ANTONIO PÉREZ , Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México D.F., México, MIGUEL CRUZ IRISSON, ESIME-Culhuacán, Instituto Politécnico Nacional, Av. Santa Ana 1000, 04430 México D.F., México — The possibility of control and modulation of the electronic properties of silicon carbide nanowires (SiCNWs) by varying the wire diameter is well known. SiCNWs are particularly interesting and technologically important, due to its electrical and mechanical properties, allowing the development of materials with specific electronic features for the design of stable and robust electronic devices. Tuning the band gap by chemical surface passivation constitutes a way for the modification of the electronic band gap of these nanowires. We present, the structural and electronic properties of fluorinated SiCNWs, grown along the [111] crystallographic direction, which are investigated by first principles. We consider nanowires with six diameters, varying from 0.35 nm to 2.13 nm, and eight random covering schemes including fully hydrogen- and fluorine terminated ones. Gibbs free energy of formation and electronic properties were calculated for the different surface functionalization schemes and diameters considered. The results indicate that the stability and band gap of SiCNWs can be tuned by surface passivation with fluorine atoms

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