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Understanding 3C-SiC/SiO_2 interfaces in SiC-nanofiber based solar cells from *ab initio* **theory**[1] TAUFIK ADI NUGRAHA, STEFAN WIPPERMANN, Max-Planck-Institute for Iron Research — Nanostructured materials – such as e. g. hybrid nanocomposites consisting of inorganic semiconducting nanofibers and organic surfactants – provide genuinely novel pathways to exceed the Shockley-Queisser limit for solar energy conversion. The synthesis of such functionalized nanofibers can be performed completely using only inexpensive wet chemical solution processing. However, the synthesis conditions often lead to complex interfacial structures involving thin oxide layers between the nanofiber and surfactants, whose atomistic details are poorly understood at best. Here we present a combined density functional theory and tight binding investigation of interfaces between 3C-SiC nanofiber surfaces and SiO_2. Considering a wide variety of possible interfacial structures we utilize a grand canonical approach to generate a phase diagram and predict the structural details of the interface as a function of the chemical potentials of Si, O and H. This study provides directions about how the synthesis conditions lead to specific types of interfacial structures and their impact on the electronic properties of the interface.

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