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First principles calculation of structural and electronic properties of the 5x5- SiC(0001) reconstructed surface[1] ALFREDO RAMIREZ, IFBUAP, Mexico and Dept. of Physics and Astr., Ohio Univ., NANCY SANDLER, Dept. of Physics and Astr., Ohio Univ., RANDALL FEENSTRA, Dept. of Physics, Carnegie Mellon Univ. — In the process of graphene layer growth via sublimation of Si atoms from SiC crystals, several reconstructions of the underlying SiC surface arise. Tunneling microscopy and spectroscopy experiments have revealed a rich spectrum of surface states in 5×5 and $6\sqrt{3} \times 6\sqrt{3} - R30^\circ$ reconstructions on the 6H-SiC(0001) surface that are important for the electronic properties of overlaying graphene layers. We have carried out a detailed study of the structural and electronic properties of the 5×5 reconstruction using Density Functional Theory methods as implemented in the SIESTA code. The model consists on a carbon adlayer that fits onto a perfect 5×5 SiC(0001) surface, with adatoms arranged with specific spatial separations. Preliminary results suggest that these reconstructions are not caused by the existence of particular stacking sequences (known as S1, S2 and S3) appearing along the c-axis during growth of the SiC crystal. The structural and electronic parameters obtained show good agreement with experimental observations and give insight into the electronic properties of graphene layers obtained with these methods.

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