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Unraveling the (3×3)-SiC($\bar{1}\bar{1}\bar{1}$) reconstruction and its role as an interface structure LYDIA NEMEC, FLORIAN LAZAREVIC[1], PATRICK RINKE, VOLKER BLUM[2], MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin — To refine the growth quality of epitaxial graphene on the C-side of SiC and improving the resulting electronic character of these films, it is important to understand the atomic and electronic-structure of the interface. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases as well as of the SiC-graphene interface is unknown. We performed a density functional theory study on the C-side of the polar SiC($\bar{1}\bar{1}\bar{1}$) surface using the all-electron numeric atom-centered basis function code FHI-aims. The formation energy of different reconstructions and model systems for the interface is presented within the thermodynamically allowed range. The surface energies of the known (2×2) phase is compared with several structural models of the (3×3) phase proposed in the literature. Inorian comparison all the previously suggested (3×3) models are higher in energy than the known (2×2) phase. We present a new model for the (3×3) reconstruction. Its formation energy crosses that of the (2×2) phase just at the carbon rich limit of the chemical potential, which explains the observed phase mixture.

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