

Abstract Submitted
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Here to stay: Stability and structure of $(6\sqrt{3}\times 6\sqrt{3})$ - $R30^\circ$ graphene on SiC(111) by all-electron DFT including van der Waals effects VOLKER BLUM, LYDIA NEMEC, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195 Berlin, Germany — SiC is a favorite growth substrate for mono- and few-layer graphene by Si sublimation. On the Si side, large ordered graphene areas can be obtained as commensurate $(6\sqrt{3}\times 6\sqrt{3})$ - $R30^\circ$ (“ $6\sqrt{3}$ ”) periodic films [1]. From a thermodynamic perspective, graphene formation competes with several other phases, including graphite on one side, and several Si-rich reconstructions on the other. The question whether $6\sqrt{3}$ graphene on SiC(111) is thermodynamically or just kinetically stabilized could be answered by density functional theory (DFT) calculations but for two challenges: (1) The needed surface slab systems are extremely large (up to 2000 atoms in this work), and (2) most standard DFT functionals do not include van der Waals effects. We here show by all-electron DFT including van der Waals effects (PBE+vdW [2]) that the $6\sqrt{3}$ graphene-like phases on SiC(111) are thermodynamically stable compared to competing surface phases, and obtain the full structure including the substrate-induced graphene corrugation. The impact of strain in smaller-cell approximants and that of possible graphene defects is discussed. [1] K. Emtsev *et al.*, Nature Materials **8**, 203 (2009). [2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

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