

Abstract Submitted  
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**The decoupling of epitaxial graphene on SiC by hydrogen intercalation: an *ab initio* study** LYDIA NEMEC, Fritz-Haber-Institut der MPG, Berlin, DE, PATRICK RINKE, Fritz-Haber-Institut der MPG, Berlin, DE; Aalto University, Helsinki, Fi, VOLKER BLUM, Duke University, Durham, NC, USA, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, DE — Large-scale ordered epitaxial graphene can be grown on various substrates, out of which silicon carbide (SiC) is one of the most promising. The exact material properties of graphene depend on the growth conditions and its interaction with the substrate. By hydrogen intercalation of epitaxial graphene on the Si-face of SiC the graphene layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [1]. We performed a density functional theory study of QFMLG on the polar 6H-SiC(0001) surface based on a van der Waals corrected semi-local exchange-correlation functional using the all-electron numeric atom-centered basis function code FHI-aims. We find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene. Using the insight gleaned on the Si-face, we present the structure of a hypothetical QFMLG phase on the C-face of SiC. We find that hydrogen intercalation is a promising option to control the SiC-graphene interface. [1] C. Riedl, *et. al*, PRL 103, 246804 (2009).

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