Abstract Submitted
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Graphene on Ru(0001): The four hills in the 25 on 23 structure THOMAS GREBER, Physik-Institut, University of Zurich, Switzerland, MARCELLA IANNUZZI, Physical Chemistry, University of Zurich, HAIFENG MA, Physik-Institut, University of Zurich, IRAKLI KALICHAVA, Swiss Light Source, Paul Scherrer Institut, HAITAO ZHOU, GENG LI, YI ZHAO, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China, STEVEN LEAKE, OLIVER BUNK, Swiss Light Source, Paul Scherrer Institut, HONJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing, JÜRG HUTTER, Physik-Institut, University of Zurich, PHIL WILLMOTT, Swiss Light Source, Paul Scherrer Institut — A single layer of sp2 hybridized carbon on Ru(0001) accommodates in a 23 on 25 superstructure with 625 carbon honeycombs as found by surface x-ray diffraction (SXRD) [1]. In a significant computational effort 25x25 unit cells of graphene were relaxed on 23x23 Ru(0001) unit cells with up to 6 substrate layers. The density functional theory calculations that take van der Waals interactions into account predict 4 protrusions, quantum dots [2] or "hills" in the unit cell with two kinds of hills: 3 Ω-type hills with a honeycomb around the summits, and one T-type hill with a single carbon atom on the summit. This prediction is confirmed by state of the art low temperature scanning tunneling microscopy and is in line with the SXRD data in Ref.[1].

[1] Martoccia et al. Phys. Rev. Lett. 101 (2008) 126102.
[2] Zhang et al. J. Phys.: Condens. Matter 22 (2010) 302001.

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None

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