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Adsorption and intercalation of Cs atoms on epitaxial graphene on Ir(111) PREDRAG LAZIC, Theoretical Physics Division, Rudjer Boskovic Institute, Bijenicka Cesta 54, Zagreb, Croatia, MARIN PETROVIC, IVA SRUT, IVO PLETIKOSIC, MILORAD MILUN, PETAR PERVAN, Institut za fiziku, Bijenicka 46, Zagreb, Croatia, SVEN RUNTE, CARSTEN BUSSE, THOMAS MICHELY, II. Physikalisches Institut, Universitat zu Koln, 50937 Koln, Zulpicher Str. 77, Germany, DAMIR SOKCEVIC, RADOVAN BRAKO, Theoretical Physics Division, Rudjer Boskovic Institute, Bijenicka Cesta 54, Zagreb, Croatia, NICOLAE ATODIRESEI, Peter Grunberg Institut (PGI-1) and Institute for Advanced Simulation (IAS- 1), Forschungszentrum Julich and JARA, 52425 Julich, Germany, JUREK SADOWSKI, ZHI-HU PAN, TONICA VALLA, Brookhaven National Lab, Upton, New York 11973, USA, MARKO KRALJ, Institut za fiziku, Bijenicka 46, Zagreb, Croatia — From the experimental studies of surface adsorption of Cs atoms and their intercalation under epitaxial graphene on Ir(111) it is known that both - adsorbed and intercalated phase of Cs atoms coexist. However, adsorbed phase is realized as a diluted superlattice adlayer of Cs atom while intercalated phase is a dense Cs layer. The preference for intercalated phase at large Cs layer densities can not be obtained from the DFT calculations with semilocal (GGA) functionals. Only after the van der Waals interaction is taken into account the agreement with experiment is achieved. From the results of calculations it follows that the main energy contribution responsible for the switching of preference from adsorption to intercalation is the graphene delamination energy from the Ir(111) surface which is dominantly of the van der Waals nature.

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