

Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Adsorption of halogenated molecule on stepped metallic surfaces: the role of van der Waals interactions RENGİN PEKOZ, KAREN JOHNSTON, DAVIDE DONADIO, Max Planck Institute for Polymer Research — The deposition of halogenated aromatic molecules on metallic surfaces is the first step for the bottom-up fabrication of atomically precise graphene nanoribbons [1]. Interest in the binding properties in this type of systems and in general in organic/inorganic interfaces has stimulated the inclusion of van der Waals (vdw) interactions within density functional theory (DFT). Using a fully non-local Van der Waals density functional (vdW-DF) [2,3] we have studied the adsorption of dichlorobenzene on stepped Au(332) and Pt(332) surfaces and on flat (111) surfaces. For several different adsorption sites, the energies, and equilibrium geometries have been computed, and electron density analysis has been performed using both conventional generalized gradient approximation (GGA) and vdW-DF. The two approaches yield qualitatively different results, highlighting the importance of non-local dispersions in this class of systems. The non-trivial role of steps edges on adsorption energies and geometries is also elucidated. [1] J. Cai *et al.*, Nature 466, 470 (2010). [2] M. Dion *et al.*, Phys. Rev. Lett. 92, 246401 (2004). [3] A. Gulans *et al.* Phys. Rev. B 79, 201105 (2009).

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Date submitted: 11 Nov 2011

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