

# Graphene on Ni(111): Strong Interaction and Weak Adsorption

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In the recent years, ab-initio modeling has been established as a complementary approach to the experimental nanoscience research. Density functional theory (DFT) based methods usually offer reliable structural models and energetics, and allow to treat systems containing several hundreds of atoms. Yet the accuracy of commonly used semi-local functionals for adsorption studies involving graphene is severely limited, as non-local (van der Waals) contributions are completely neglected. In a recent publication [1], we could demonstrate that the evaluation of the correlation energy in a many-electron approach based on the adiabatic-connection fluctuation-dissipation theorem (ACFDT) in the random phase approximation (RPA) leads to a significant improvement.

In this presentation, I will discuss our recent results [2] for the adsorption of graphene on Ni(111) on the basis of RPA calculations. Although we find a significant hybridization between the graphene  $\pi$  orbitals and Ni  $d_{z^2}$  states at an optimized binding distance of 2.17 Å, the adsorption energy is still in the range of a typical physisorption (67 meV per carbon). An important contribution to the energy is related to an decrease in the exchange energy resulting from the adsorption-induced lower symmetry in the graphene layer. The energetics can be well reproduced using the computationally significantly cheaper van der Waals density functional theory (vdW-DF) with an appropriately chosen exchange-correlation functional.

[1] L. Schimka, J. Harl, A. Stroppa, et al., *Nature Materials* 9 (2010) 741.

[2] F. Mittendorfen, A. Garhofer, J. Redinger, J. Klimeš, J. Harl, and G. Kresse, *submitted*