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Ni(111)-graphene interface: the importance of screened van der Waals interactions PIER LUIGI SILVESTRELLI, ALBERTO AMBROSETTI, Università degli Studi di Padova — Due to the direct applicability of Ni(111) surfaces in high-quality graphene production, the Ni(111)-graphene interface has recently been the object of extensive experimental and theoretical investigations. Achieving an accurate and efficient theoretical description of the Ni(111)-graphene interaction, however, still represents a major theoretical challenge, due to the complex interplay between van der Waals (vdW) and hybridization effects. Here we apply the DFT/vdW-WF2s method [1], augmenting semi-local Density Functional Theory through the inclusion of screened vdW interactions. Interestingly, we show that a reliable description of the vdW energy in Ni(111)-graphene requires an appropriate modeling of the metal-screening, which should not only account for the p- and s-like *quasi-free* electrons, but should further include the effect of the more *localized* d-like states. Good agreement is found with experiment and highly accurate theoretical predictions. Moreover, being the DFT/vdW-WF2s method based on Maximally Localized Wannier Functions, it permits an intuitive understanding of the complex physics underlying transition metals-graphene interactions.

[1] P. L. Silvestrelli and A. Ambrosetti, Phys. Rev. B 87, 075401 (2013).

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