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Transition metals-graphene interaction: the role of the screened van der Waals energy ALBERTO AMBROSETTI, PIER LUIGI SILVESTRELLI, Università degli Studi di Padova — The interaction of graphene with transition metals is of particular interest for practical applications, which include for instance the efficient production of high-quality graphene. The accurate theoretical description of transition metals-graphene interfaces, however, is a particularly challenging problem due to the complex interplay between van der Waals (vdW) and hybridization effects. Here we apply the DFT/vdW-WF2s method [1], which allows to augment semi-local Density Functional Theory through the introduction of screened vdW interactions. Notably, we find that a reliable modeling of the van der Waals interaction should account for complex metal screening effects, that are due to the combined contributions of the p- and s-like *quasi-free* electrons, and the more *localized* d-states. The resulting geometry and energetic properties are in good agreement with experimental data and sophisticates theoretical calculations. Moreover, the Maximally Localized Wannier Functions underlying the DFT/vdW-WF2s method allow for an intuitive understanding of the complex binding mechanism.

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

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