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Chemical Trends for Transition Metal Compound Bonding to Graphene BJOERN LANGE, VOLKER BLUM, Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC, USA — Transition metal compounds are of interest as catalysts for the hydrogen evolution reaction (HER). However, a perfect candidate to replace expensive platinum has not yet been identified. To tailor a specific compound, several properties come into play. One is the bonding to the underlying substrate, for which π-bonded carbon nanostructures are promising candidates. Here we analyze the bonding of small transition metal compound nanoclusters to a graphene layer for a range of chemical compositions: M_xA_y (M = Mo, Ti; A = S, O, B, N, C). The clusters are generated by an unbiased random search algorithm. We perform total energy calculations based on density functional theory to identify lowest energy clusters. We calculate binding energies using the PBE and HSE functionals with explicit van der Waals treatment[1] and benchmark those against RPA cluster calculations. Our results indicate that molybdenum-carbides and -nitrides tend to bond tightly to graphene. Mo-oxides and -sulfides show small binding energies, indicating van der Waals bonding.

[1] Tkatchenko, A., Scheffler, M., PRL **102**, 073005 (2009)

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