

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Transport properties of metallo-organic functionalized graphene¹

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NRL, Washington, DC — Transition metal atoms can act as strong covalent anchors for organic molecules on graphene. The hybridization between the metallic d orbitals and the p orbitals of graphene provides a doping method without breaking C-C bonds. Using first-principle calculations for a range of adsorbed transition metals we identify the induced impurity levels and we reveal a dependence of the spin states on adsorbate coverage. We construct sets of maximally localized Wannier functions that interpolate accurately the calculated bandstructures. These sets are used then to describe the electronic transport from the dilute regime to finite coverages.

¹This work was supported in part by ONR.

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Date submitted: 30 Dec 2010

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