

Abstract Submitted
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Rigid band shifts, charge pinning, and charge transport through graphene junctions with wetting metal contacts TOBIAS BOTHWELL, SALVADOR BARRAZA-LOPEZ, University of Arkansas — It is a common perception that graphene band shifts cannot be determined directly when attached to chemisorbed (“wetting”) metals due to the hybridization of graphene bands around the Dirac point. Graphene has deeper energy (sigma) bands which don’t hybridize with the metal’s bands, providing a definite measure of actual shifts. Looking at hybridization in a controlled way (by varying the metal/graphene separation by hand) one realizes the shifts can actually be considered rigid, i.e., σ - and p - bands shift by about the same energy Δ_E . In a related context, charge depinning is the modification of graphene’s electron density at a metal/graphene interface with a (back) gate. Depinning happens at metal/graphene interfaces with physisorbed (non-wetting) metals. Oxidation or contamination at the interface can lead to charge depinning as well. Using first-principles calculations, we establish a link between charge depinning at a wetting metal/graphene interface and the quality of such an interface. For this purpose, metal/graphene/insulator structures are studied under transverse bias. We also report transmission coefficients through nanoscale two-terminal graphene/metal junctions.

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