Screening and electrostatic doping in multilayer graphene systems

MARCELO KURODA, J. TERSOFF, RAZVAN NISTOR, GLENN MARTYNA, IBM TJ Watson Research Center — We study the electrostatic screening in multilayer graphene systems using ab initio calculations and analytical models. First principles calculations reveal that oriented (Bernal) and turbostratic graphene multilayers in contact with a metal slab show only small differences in their charge distribution despite their dissimilar electronic structure. In the turbostratic systems the layer decoupling enables the identification of the Dirac point for each individual layer. We then measure the shift of each Dirac point relative to the Fermi level of the system and compute the charge transfer to each layer. Results are compared with an analytical model considering discrete layers. The model shows that at \( T = 0 \) charge screening is highly nonlinear due to the vanishing density of states at the Fermi level. More importantly a strong dependence on charge and temperature results in a change of the screening length by more than an order of magnitude depending on the experimental conditions, reconciling the large range of screening lengths previously reported in experiments.