Dielectric susceptibility of graphene due to its out-of-plane polarizability

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Although atomically thin, graphene monolayer has a significant out-of-plane polarizability that is important for self-consistent quantitative analysis of gating of both Bernal-stacked and twisted graphene multilayers. The out-of-plane electric field is screened by both the charge redistribution among the layers and by polarizability of orbitals in each of the layers. We show how to consistently implement both screening mechanisms, taking into account that layers are not polarized by the field from their own charges, Fig.1. For bilayer this leads to the equation (see Fig 1 for the notations):

$$U_t - U_b = \frac{e\,d}{\epsilon_0}\left[\frac{D}{\epsilon_z} - e\,\frac{1+\epsilon_z{}^{-1}}{2}\left(\frac{n_b - n_t}{2}\right)\right].$$

To determine ϵ_z, we combine the DFT analysis of out-of-plane polarizability of monolayer graphene, producing $\epsilon_z = 2.65$, with the available experimental data [3-5], fitted with self-consistent tight-binding model calculations of electronic band structure in electrically gated Bernal-stacked and twisted bilayers, Fig.2. Upon comparison, we find a good agreement with the theoretically computed $\epsilon_z = 2.65$.

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FIGURES

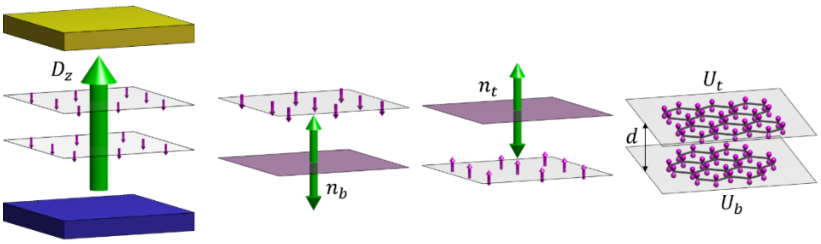

Figure 1: Dielectric polarisation of graphene layers, induced by external displacement field [left panel] and by the charges on the bottom and top layers [two central panels]. Right: Notations for layer potentials.

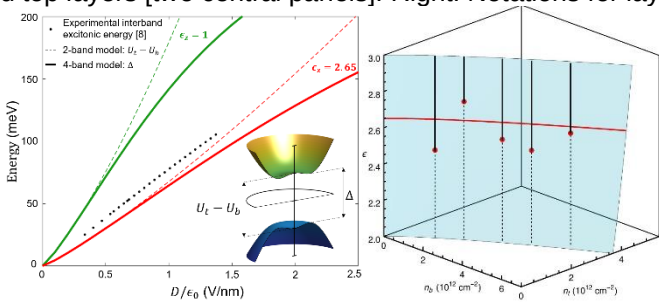

Figure 2: Left: Calculated gap in Bernal graphene bilayer compared with exciton spectrum measured in [4]. Right: Calculation of layer densities for single-gated twisted graphene bilayer (cyan surface) is compared with experiment [2] (black lines) for different values of ϵ_z.