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Ab-initio study of polarization in graphene films ERIC YU, Department of Electrical and Computer Engineering, Cornell University, DEREK STEWART, Cornell Nanoscale Facility, Cornell University, SANDIP TIWARI, Department of Electrical and Computer Engineering, Cornell University — We present an ab-initio analysis of polarization of multilayer graphene systems under applied electric fields. The effects of applied electric fields are calculated using a Berry phase approach with a plane-wave density functional formalism. We have determine polarizability values for graphene films and carbon nanotubes and find that the polarizability of graphene films follows a linear relationship with the number of layers. We also examined changes in the induced charge distribution as a function of graphene layers. We focus in particular on bilayer graphene and find that the induced charge accumulates primarily on the B sublattice sites. This induced charge distribution was also confirmed by a separate tight-binding Green's function calculation.

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