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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 determined 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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