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Carrier Density Modulation in the Graphene/Ferroelectric Interface[1] DIOMEDES SALDANA-GRECO, University of Pennsylvania, CHRISTOPH BAEUMER, MOONSUB SHIM, LANE W. MARTIN, University of Illinois at Urbana-Champaign, ANDREW M. RAPPE, University of Pennsylvania — Atomic and electronic structure insights of the graphene/ferroelectric interface via density functional theory (DFT) calculations elucidate the yet unexplored theoretically anticipated strong coupling between graphene transport properties and the exposed ferroelectric polarization. A model system consisting of ferroelectric $LiNbO_3$ (0001) slab with graphene facing both up- and down-polarized surfaces has been constructed to investigate the nature of the interfacial interaction. Our DFT calculations predict that the electronic structure of graphene facing either polar surface is preserved with neat Dirac cones at the K points in the Brillouin zone. We observed that the Dirac cone of the graphene in close contact with the up-polarized (down-polarized) $LiNbO_3$ surface is shifted below (above) the Fermi energy. Here, we demonstrate experimentally and theoretically that the doping levels of graphene can be modulated based on the ferroelectric polarization, temperature-induced potential inversion and surface reconstructions leading to increased and decreased electron concentration in graphene on up-polarized and down-polarized $LiNbO_3$ surfaces, respectively.

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