Title

Giant Effective charges and Piezoelectricity in Gapped Graphene

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abstract

A single layer of ideal graphene is an homopolar material, with vanishing infrared (IR) effective charges and piezoelectricity. In contrast graphite and multilayered graphene can present a significant IR activity. Here we demonstrate, by combining ab-initio calculations and analytical modeling, how symmetry breaking mechanisms that open a band gap in the graphene electronic-structure can also activate a huge IR and/or a piezoelectric response [1]. In particular, the piezoelectric coefficient per layer in gapped graphene is 3 times that of Boron Nitride and 30% larger than that of and Molybdenum Disulfide. By relating the IR charges and piezoelectric coefficient to the valley Chern number, we explain why such quantities are independent of the magnitude of the band gap for band gap smaller than 0.5 eV. The predicted large values of piezoelectric coefficient and dynamical effective charge can significantly influence the electron-phonon scattering processes, and thus charge transport and the relaxation-dynamics of photo-excited carriers. We acknowledge financial support by the European Graphene Flagship Core 2 grant number 785219.

[1] O. Bistoni, P. Barone, E. Cappelluti, L. Benfatto, F. Mauri, 2D Mater. 6 045015 (2019)