

Abstract Submitted
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Tunable Optoelectronic Properties of Semiconducting Graphene¹

MARC DVORAK, ZHIGANG WU, Department of Physics, Colorado School of Mines — If patterned properly, structural modifications on graphene can induce intervalley scattering between Dirac points and open a sizeable band gap. Such two-dimensional semiconductors could offer great tunability in electronic and optical properties. We performed calculations based on many-body perturbation theory using Green's functions to obtain quasiparticle energies and optical absorption spectra for these semiconducting graphene structures, focusing on the role of defect size, type, and geometric configuration. Our results show a strong renormalization of the band gap over Kohn-Sham energy levels and exciton binding energies greater than 0.4 eV. By stacking monolayer defected graphene with various defect sizes and configurations, one could create an excellent photovoltaic absorber layer that efficiently absorbs photons with energy larger than 1.0 eV.

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