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作者: Chen, JZ (Chen, Jingzhe); Hu, YB (Hu, Yibin); Guo, H (Guo, Hong)
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摘要: We report on a first-principles investigation of photocurrent generation by graphene PN junctions. The junctions are formed by either chemically doping with nitrogen and boron atoms, or by controlling gate voltages. The nonequilibrium Green's function formalism combined with density functional theory is applied to calculate the photoresponse function. The graphene PN junctions show a broadband photoresponse including the terahertz range. The dependence of the response on the angle between the light polarization vector and the PN interface is determined. Its variation against photon energy E-ph is calculated in the visible range. The essential properties of chemically doped and gate-controlled PN junctions are similar, but the former shows fingerprints of dopant distribution.
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地址: [Chen, Jingzhe] McGill Univ, Ctr Phys Mat, Montreal, PQ H3A 2T8, Canada
McGill Univ, Dept Phys, Montreal, PQ H3A 2T8, Canada
通讯作者地址: Chen, JZ (通讯作者),McGill Univ, Ctr Phys Mat, Montreal, PQ H3A 2T8, Canada
电子邮件地址: chenj@physics.mcgill.ca
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