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Accession number:12658985
Title:First-principles analysis of photocurrent in graphene P N junctions
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Source title:Physical Review B (Condensed Matter and Materials Physics)
Abbreviated source title:Phys. Rev. B, Condens. Matter Mater. Phys. (USA)
Volume:85
Issue:15
Publication date:15 April 2012
Pages:155441 (6 pp.)
Language:English
ISSN:1098-0121
CODEN:PRBMDO
Document type:Journal article (JA)
Publisher:American Physical Society
Country of publication:USA
Material Identity Number:DQ91-2012-015
Abstract:We report on a first-principles investigation of photocurrent generation by graphene P N 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 P N 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 P N junctions are similar, but the former shows fingerprints of dopant distribution.
Number of references:33
Inspec controlled terms:ab initio calculations - boron - density functional theory - doping profiles - graphene - Green's function methods - light polarisation - nitrogen - photoconductivity - photoemission
Uncontrolled terms:first principles analysis - photocurrent - graphene P N junctions - doping - gate voltage - nonequilibrium Green's function - density functional theory - photoresponse function - light polarization vector - photon energy - dopant distribution - C:N - C:B
Inspec classification codes:A7960 Photoemission and photoelectron spectra (condensed matter) - A7240 Photoconduction and photovoltaic effects; photodielectric effects - A7360T Electrical properties of fullerenes and related materials (thin films/low-dimensional structures) - A7115A Ab initio calculations (condensed matter electronic structure) - A7115P General mathematical techniques in electronic structure calculations (condensed matter) - A7115M Density functional theory, local density approximation (condensed matter electronic structure) - A7865V Optical properties of fullerenes and related materials (thin films/low-dimensional structures) - A6170W Impurity concentration, distribution, and gradients
Chemical indexing:C:N/bin C/bin N/bin C/el N/el N/dop;C:B/bin B/bin C/bin B/el C/el B/dop
Treatment:Theoretical or Mathematical (THR); Experimental (EXP)

Discipline:Physics (A)
DOI:10.1103/PhysRevB.85.155441
Database:Inspec