Doping induced Rashba spin splitting in graphene and planar boron nitride

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Motivation

Graphene – hope for future electronic and spintronic devices

⊕ The first material to demonstrate room temperature spin transport

⊕ Very long spin lifetime owing to extremely small spin-orbit coupling

⊖ Too small spin splitting, not favorable for spin FET

Method

Density Functional Theory (DFT)

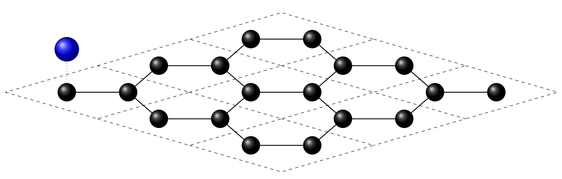
Fully relativistic calculation

Pseudopotentials: PAW (projector augmented wave), TM (Troullier – Martins)

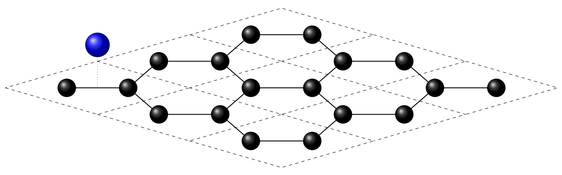
Codes used: VASP, our own

Geometry of decorated graphene and planar boron nitride

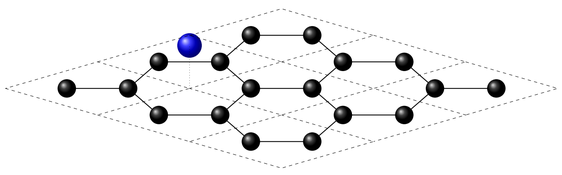
3×3 super-cell with ad-atom on the TOP:



3×3 super-cell with ad-atom on the BRIDGE:



3×3 super-cell with ad-atom in the HOLLOW:



Results – geometry of decorated graphene

Equilibrium positions of ad-atoms in graphene:

Ad-atom	Super-cell	Nr of matrix atoms	Position	Ad-atom height [A]
Ge	1×1	2	TOP	3.602
	2×2	16	TOP	2.156
	4×4	32	TOP	2.156
Sn	1×1	2	TOP	3.822
	2×2	16	TOP	2.621
	4×4	32	TOP	2.401
Ca	1×1	2	HOLLOW	2.083
	2×2	16	HOLLOW	2.205
	4×4	32	HOLLOW	2.205

One ad-atom in $n \times n$ superlattice:

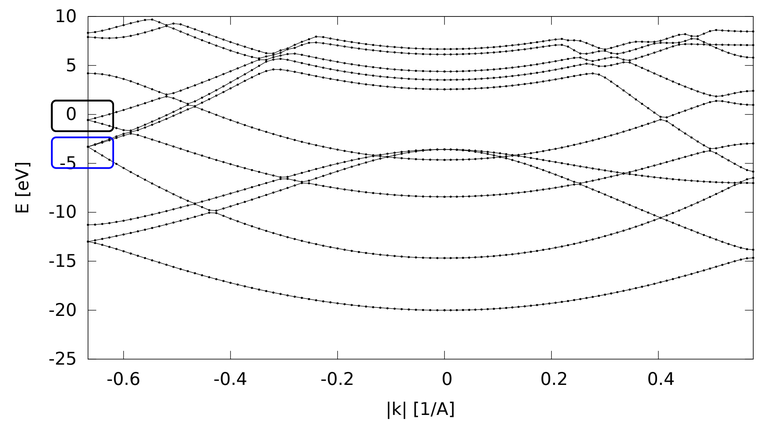
$$concentration[\%] = \frac{100}{(2 \times n^2)} \qquad (1)$$

Results – geometry of decorated boron nitride

Example – equilibrium system energies in boron nitride (BN), different possible ad-atom positions:

Ad-atom	Super-cell	Position	Ad-atom height [A]	E_{tot} minimum [eV]
Ge	2×2	TOP	2.814	−78.157
	2×2	HOLLOW	2.714	−78.183
	2×2	BRIDGE	2.615	−78.182

Results – Ge decorated graphene full $K - \Gamma - M$ band structure



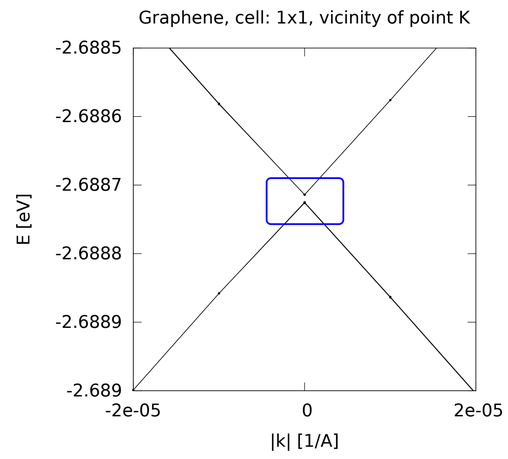
Two bands of atomic carbon p_z character

Two bands of atomic germanium p_x-p_y character and one band of atomic germanium s character

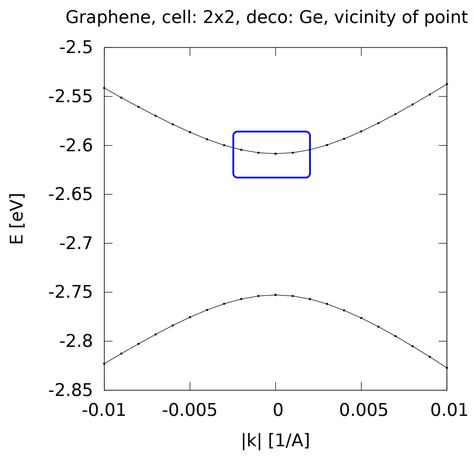
Results – modifications of Dirac cone in graphene

Three cases:

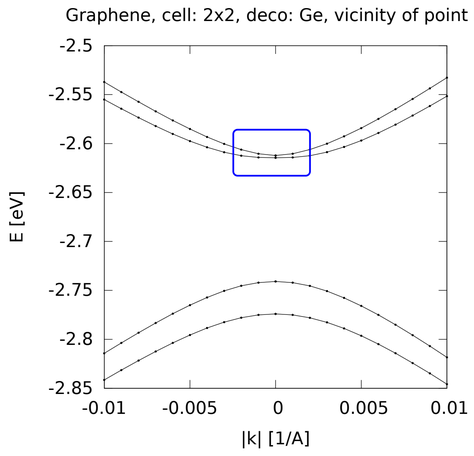
- Fully relativistic calculation of pure graphene. Bands remain doubly degenerated, four-fold degeneration in point K vanishes!



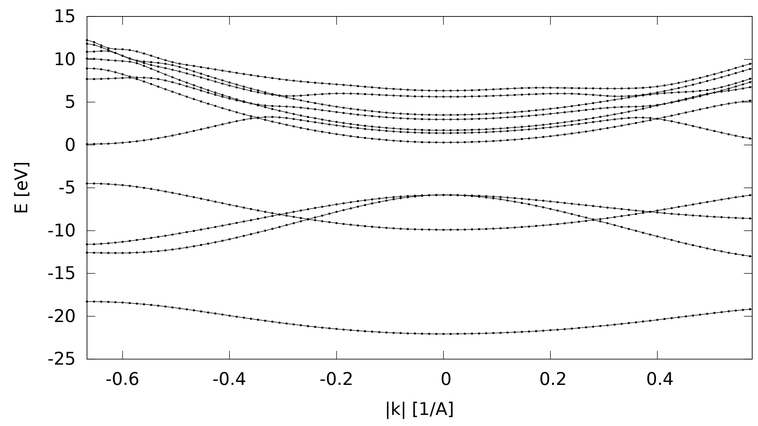
- Scalar relativistic (no spin-orbit included) calculation of graphene decorated with Ge atoms. Bands are parabolic now and remain doubly degenerated.



- Fully relativistic (spin-orbit included) calculation of graphene decorated with Ge atoms. Double degeneration of bands vanishes.

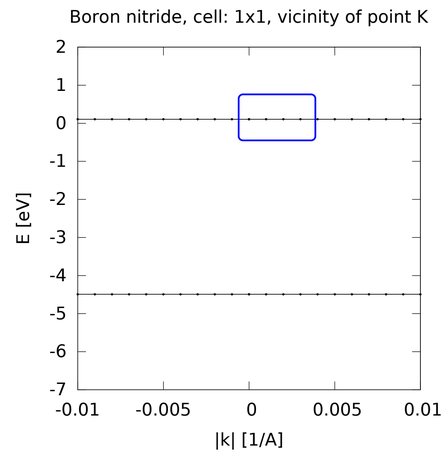


Results – boron nitride full $K - \Gamma - M$ band structure

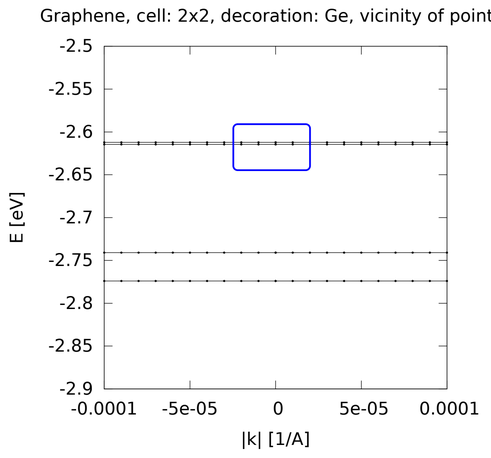


Results – boron nitride vicinity of point K

Fully relativistic calculation of boron nitride.
Bands are parabolic and remain doubly degenerated.



Results – Ge decorated graphene very vicinity of point K



Results – energy differences

System	Spin-orbit	Gap_{cone}	Δ_c	Δ_v
1×1 graphene + Ge	-	0.012	–	–
1×1 graphene + Ge	+	0.011	0.001	0.000052
2×2 graphene + Ge	-	0.14	–	–
2×2 graphene + Ge	+	0.16	0.0023	0.033
1×1 graphene + Sn	-	0.027	–	–
1×1 graphene + Au	-	0.0004	–	–

Summary and outlook

Ab initio calculations clearly demonstrate that the spin splitting of bands in graphene can be modified by decorating the layers with heavier atoms.

Further studies of the electronic structure of graphene with various decorating atoms (Pb) and molecules.

Modeling of the growth process (chemical reactions) that could lead to effective incorporation of adatoms.

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