Intrinsic and extrinsic spin-orbit coupling in monolayer nitrogene.

Paulina Jureczko*, Marcin Kurpas[1]

[1] *Institute of Physics, University of Silesia in Katowice, ul. 75 Pułku Piechoty 1, 41-500 Chorzów*

* *paulina.jureczko@us.edu.pl*

Monolayer nitrogene was recently predicted to be stable two-dimensional material even far above the room temperature [1]. It is an indirect gap nonmagnetic insulator, with the gap of 4 eV [1]. Nitrogene crystallizes in a centrosymmetric buckled honeycomb lattice, similar to other graphene analogues, such as, silicene, blue phosphorene or arsenene [2,3]. Although the electronic, mechanical and thermal properties of nitrogene have been studied by several authors [1,4–6], the spin-orbital effects have not been studied in detail yet. Here, we perform a systematic theoretical study of the spin-orbit coupling in this material. Specifically, we employ first-principles methods to obtain the basic orbital and spin-orbital properties of nitrogene, also in the presence of an external transverse electric field. We calculate the spin-mixing parameter b^2 and spin-orbit fields Ω to extract essential information about the intrinsic and extrinsic spin-orbit coupling in the band structure.
We find, that the values of b^2 are very small, on the order of 10^{-6}, similar to those of graphene [7]. The values of $\hbar\Omega$ are below $1\,\mu eV$ for E=1 V/nm. Our results show, that even if nitrogene is a heavier element than carbon, the effective spin-orbit coupling in the bands close to the band gap is weaker for nitrogene than for graphene, due to the specific topology of the band structure.

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