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Electronic structure of graphitic nanocone influenced by spin-orbit coupling and boundary effects

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The graphene-based nanostructures can be derived from graphene by adding the topological defects into the hexagonal carbon structure. In this way, the graphitic nanocone could be fabricated using different numbers of the pentagons.

The spin-orbit coupling in the graphitic nanocone seems to be quite strong, much stronger than in the plain graphene. This effect is caused by the curvature of this material and it could contribute to the present progress in the areas of spintronics and straintronics. Furthermore, because of the overlap of the atomic orbitals close to the tip of the nanocone, boundary effects influence the electronic structure of the material: the interaction of the opposite atoms which we call the pseudopotential and of the π-orbitals of the neighbouring atoms. It seems that for a suitable vortex angle, a significant localization of the electrons in the tip appears. This effect could have a good potential use as a microscope probe in atomic force microscopy.

Different methods could be used for the calculation of the electronic structure: the base step is the tight-binding method which enables to calculate the energy spectrum from the matrix of the Hamiltonian. This method is valuable for case of a simple [1]. For the inclusion of the supplementary effects, we use the gauge field-theory approach in which a Dirac-like equation on the 2-dimensional molecular surface is solved. The spin-orbit coupling and the pseudopotential are present by the corresponding terms in this equation [2,3]. The resulting wave-function we use for the calculation of the local density of states. For the more precise calculation of the energy levels, the Green function method could be also applied.

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