LUT University

Gate-tunable magnetism of C adatoms on graphene

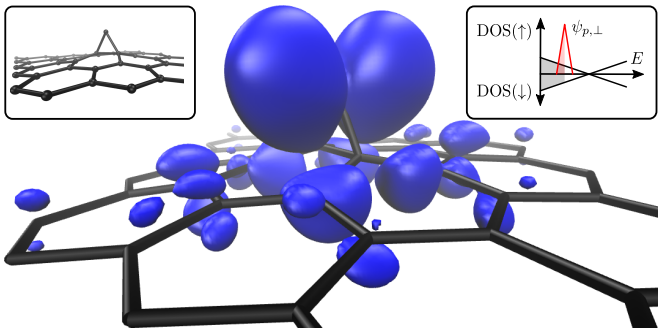

FIG. 1. Magnetization density isosurface plot for a C adatom on graphene. The isosurface is at $0.004\,e/\text{Å}^3$, while the corresponding negative isosurface is not visible. The $\psi_{p,\perp}$ state (with p_x/p_y-symmetry) is visible at the adatom. Its p_z character on the graphene sheet can be seen as well. Left inset: another view of the geometry. Right inset: schematic electronic structure, the occupied portion of the graphene/$\psi_{p,\perp}$ states are in gray/red, respectively.

We have performed density functional theory calculations of graphene decorated with carbon adatoms, which bind at the bridge site of a C–C bond. Earlier studies have shown that the C adatoms have magnetic moments and have suggested the possibility of ferromagnetism with high Curie temperature. Here we propose to use a gate voltage to fine tune the magnetic moments from zero to $1\,\mu_\text{B}$ while changing the magnetic coupling from antiferromagnetism to ferromagnetism and again to antiferromagnetism. These results are rationalized within the Stoner and RKKY models. When the SCAN meta-GGA correction is used, the magnetic moments for zero gate voltage are reduced and the Stoner band ferromagnetism is slightly weakened in the ferromagnetic region.

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[1] J. Nokelainen, I. V. Rozhansky, B. Barbiellini, E. Lähderanta, and K. Pussi, arXiv e-prints , arXiv:1805.06044 (2018), arXiv:1805.06044 [cond-mat.mes-hall].