EXCHANGE INTERACTION BETWEEN COBALT AD-ATOMS ON ZIGZAG- EDGE GRAPHENE NANORIBBON

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Based on LSD spin polarized calculations, we compare parallel and antiparallel ordering of moments of pairs of Co impurities in graphene zigzag-edge nanoribbon. Different locations with respect to nanoribbon edges are considered. The space dependence of magnetic moment distribution and local distortions are calculated. The adatom induced curvature is observed for narrow ribbons. Exchange interaction is strongly anisotropic mainly due to the existence of electron edge states. For infinitely long nanoribbons the presence of a gap in the energy spectrum results in superexchange-type exchange mechanism, whereas for finite length or for doped nanoribbons the dominate mechanism is RKKY-like. The calculations are performed employing VASP package with the projector augumented wave basis and making use of generalized gradient approximation.

-13.4 cm -

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 $9.7~\mathrm{cm}$