Quantum chemical calculations of carbon nanoscroll energy rolled from zigzag graphene nanoribbon

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Using the semi-empirical quantum chemical PM3 method the energies of carbon nanoscrolls formed from flat zigzag graphene nanoribbons 46zGNR and 70zGNR are calculated. For this purpose a simple algorithm to define the Cartesian coordinates of the atoms of a carbon nanoscroll is proposed. The dependences of the energy of the nanoscrolls relative to the energy of the corresponding flat nanoribbon on the inner radius of nanoscroll obtained using both the quantum chemical calculations and the semi-classical analytical model shows the bistability of the system. This shows promise for nanoscroll-based nanoelectromechanical systems.

Keywords: carbon nanoscroll, graphene nanoribbon, Archimedean spiral, Cartesian coordinates.

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