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CONTROLLED FORMATION OF CARBON NANOSTRUCTURES THROUGH DEFECT ENGINEERING IN GRAPHENE

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Using numerical simulations we demonstrate the spontaneous formation of various 3D carbon nanostructures, like multi-tube carbon nanotubes, nanopyramids, nanocubes, artificially rippled graphene, and other exotic nanomaterials, starting from graphene nanoribbons and inducing controllably engineered defects consisting of carbon adatoms or inverse Stone-Wales defects. The evolution of the initial defected planar structures towards the final 3D nanoarchitectures is obtained through molecular dynamics simulations, using different force fields to ensure the reproducibility of the derived results [1].

It has been shown that periodic arrays of appropriate structural defects produce a stable and controllable inflection of a graphene sheet. This effect was used to obtain a variety of carbon nanotubes with different chiralities and sizes [2]. Lines of defects applied at the top or bottom side of graphene result in downward or upward, respectively, inflection of the sheet. Therefore, spatially designed defect distributions in graphene can spontaneously form a large variety of stable 3D nanostructures, of controllable size and shape, on demand.

The presented carbon nanostructures of different shapes, sizes, and morphologies, can be used in applications ranging from storage of hydrogen or other molecules, enhanced chemical reactions or catalysis in confined compartments, to drug delivery nanodevices and biosensors.

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References:

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