Modelling of 3D Nanographene

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In the low-density regime of carbon materials, nanoporous formation along with nanostructuring and coexistence of various hybridizations give rise to three-dimensional (3D) structures with outstanding properties. Carbon nanofoams (CNFs) belong to this class of materials. They are open, random and light structures resembling a foam. We have recently studied [1]. CNFs made up of schwarzites, nanostructures with negative Gaussian curvature. Here, we investigate another form of this exciting material - the 3D Nanographene (3D-NG) - which is made of graphene nanoflakes. This 3D randomly interconnected structure offers an alternative route for promising applications. Our studies are based on Monte Carlo simulations for the network formation, followed by tight-binding molecular dynamics simulations for full relaxation and calculation of the mechanical and optoelectronic properties. We find that 3D-NG is rigid, despite its porous nature, so it can be utilized in applications (catalysis, tribology, energy storage) as thin films. It, also, exhibits high conductivity, approaching that of single-layer graphene, and high optical absorptivity. Similar properties are exhibited by the CNT foams. This makes this 3D manifestation invaluable for applications in electronics and optics.

References

[1] C. Mathioudakis and P. C. Kelires, Phys. Rev. B **87**, 195408 (2013).

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