Physical Properties of Twin Sun Graphene: A Density Functional Theory Study

Roya Majidi[1,*]

[1] *Department of Physics, Shahid Rajaee Teacher Training University, Lavizan, 16788-15811 Tehran, Iran*

A new sheet with the name twin sun graphene composed of 4- and 8-membered rings is suggested. The structural, mechanical, electronic, and optical properties of C twin sun graphene and twin sun graphene-like BN sheets are studied by using density functional theory. These sheets exhibit dynamic stability as well as good energetic and thermal stability, especially at room temperature. The C and BN twin graphene sheets are softer and more prone to deformation compared to graphene, so they have the potential to be used particularly when softer materials than graphene are required. The C twin sun graphene shows semiconductor properties, while the BN twin sun graphene is an indirect band gap insulator. An anisotropic behavior for the optical properties of the sheets is observed. Due to their high dielectric constants, and optical absorption, particularly in the ultraviolet region, they sheets could be able to store energy and filter out harmful ultraviolet radiation. These nanosheets are well-suited for use in nano-mechanics and nano-optoelectronics due to their favorable mechanical, electronic, and optical characteristics.

* E-mail addresses: r.majidi@sru.ac.ir, royamajidi@gmail.com
ORCID: 0000-0001-8451-3695