Graphene foams, pillared graphene frameworks and low density 2D carbon allotropes: a computational overview

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Abstract

Graphene is one of the most studied carbon allotropes with fascinating properties and several possible striking applications, ranging from electronic to mechanical ones. We present a set of molecular dynamics studies aimed to characterize 3D graphene structures such as graphene nanofoams [1], of which we assess the thermal and mechanical properties, and pillared graphene frameworks [2], porous materials suitable for gas adsorption and separation. Furthermore, we present novel three-coordinated 2D carbon allotropes obtained by means of an augmentation procedure applied to uniform planar tessellations [3]. We assess the mechanical and electronic properties of these materials from ab-initio calculations. A significant lowering of areal density has been obtained possibly reaching the lowest density within the set of three-coordinated, locally-jammed, periodic structures.

References


Figures

Figure 1: Graphene random foam. We present the modeling and assessment of the properties of these materials.

Figure 2: Pillared graphene frameworks are porous structures made of graphene layers intercalated by organic moieties.

Figure 3: Augmentation of a tiling (the octa-square tiling here) as method to decrease the area density.