Название публикации:
Using spiral chain models for study of nanoscroll structures

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Сведения об издании:
PHYSICAL REVIEW B
Том: 97 Выпуск: 16
Номер статьи: 165436
DOI: 10.1103/PhysRevB.97.165436
Опубликовано: APR 26 2018
Тип документа: Article

Аннотация:
Molecular nanoribbons with different chemical structures can form scrolled packings possessing outstanding properties and application perspectives due to their morphology. Here, we propose a simplified two-dimensional model of the molecular chain that allows us to describe the molecular nanoribbon's scrolled packings of various structures as a spiral packaging chain. The model allows us to obtain the possible stationary states of single-layer nanoribbon scrolls of graphene, graphane, fluorographene, fluorographane (graphene hydrogenated on one side and fluorinated on the other side), graphone C4H (graphene partially hydrogenated on one side), and fluorographone C4F. The obtained states and the states of the scrolls found through all-atomic models coincide with good accuracy. We show the stability of scrolled packings and calculate the dependence of energy, the number of coils, and the inner and outer radius of the scrolled packing on the nanoribbon length. It is shown that a scrolled packing is the most energetically favorable conformation for nanoribbons of graphene, graphane, fluorographene, and fluorographane at large lengths. A double-scrolled packing when the nanoribbon is symmetrically rolled into a scroll from opposite ends is more advantageous for longer length nanoribbons of graphone and fluorographone. We show the possibility of the existence of scrolled packings for nanoribbons of fluorographene and the existence of two different types of scrolls for nanoribbons of fluorographane, which correspond to the left and right Archimedean spirals of the chain model. The simplicity of the proposed model allows us to consider the dynamics of molecular nanoribbon scrolls of sufficiently large lengths and at sufficiently large time intervals.

Ключевые слова:
Carbon nanoscrolls; mechanical-properties; graphene nanoribbons; molecular-dynamics; simulation; fabrication; graphite; scrolls; md