Название публикации:
Two-Dimensional Model of Scrolled Packings of Molecular Nanoribbons

Авторы:
Savin, AV [1,2] ; Mazo, MA [1]

[1] Russian Acad Sci, Semenov Inst Chem Phys, Moscow 119991, Russia
[2] Plekhanov Russian Univ Econ, Moscow 117997, Russia

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Аннотация:
A simplified model of the in-plane molecular chain, allowing the description of folded and scrolled packings of molecular nanoribbons of different structures, is proposed. Using this model, possible steady states of single-layer nanoribbons scrolls of graphene, graphane, fluorographene, and fluorographane (graphene hydrogenated on the one side and fluorinated on the other side) are obtained. Their stability is demonstrated and their energy is calculated as a function of the nanoribbon length. It is shown that the scrolled packing is the most energetically favorable nanoribbon conformation at long lengths. The existences of scrolled packings for fluorographene nanoribbons and the existence of two different scroll types corresponding to left- and right-hand Archimedean spirals for fluorographane nanoribbons in the chain model are shown for the first time. The simplicity of the proposed model makes it possible to consider the dynamics of scrolls of rather long molecular nanoribbons at long enough time intervals.

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