

Название публикации:

Edge Vibrations of Graphane Nanoribbons

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Сведения об издании:

PHYSICS OF THE SOLID STATE

Том: 60 Выпуск: 5 Стр.: 1046-1053

DOI: 10.1134/S1063783418050281

Опубликовано:МАУ 2018

Тип документа:Article

Аннотация:

Using the COMPASS force field, natural linear vibrations of graphane (graphene hydrogenated on both sides) nanoribbons are simulated. The frequency spectrum of a graphane sheet consists of three continuous intervals (low-frequency, mid-frequency, and narrow high-frequency) and two gaps between them. The construction of dispersion curves for nanoribbons with a zigzag and chair structure of the edges show that the frequencies of edge vibrations (edge phonons) can be present in the gaps of the frequency spectrum. In the first type of nanoribbons, two dispersion curves are in the low-frequency gap of the spectrum and four dispersion curves in the second gap. These curves correspond to phonons moving only along the nanoribbon edges (the mean