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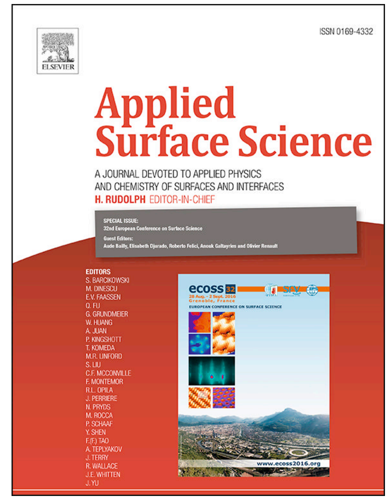

Full Length Article

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Curvature And Vacancies In Graphene Quantum Dots

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Highlights:

Optical and geometric features of multivacancy GQDs were studied using DFT calculations.

Square and pentagonal figures are important in the properties of such materials.

The configuration of the multivacancy is key for the geometric structure.

The differences between vacancies in graphene are likely to be related to non-periodicity.

Abstract

The optical properties and the geometric characteristics of multivacancy graphene quantum dots systems are studied using Density Functional Theory calculations, in a systematic way, in relation to the number of carbon atoms extracted and the relative configurations that could be present in the cluster. The way to characterize these configurations was using the complementary figure model –i.e. the figure formed by the carbon atoms extracted in order that the vacancy could be created-. The number of pentagonal or square figures formed after structure optimization, as well as their relative location, is found to be very relevant to determine the curvature level of the graphene quantum dot, but the occurrence of higher order cycles have a non-negligible role and cannot be ruled out. However, this occurrence is much dependent on the specific multivacancy to be studied and prevents to reach more accurate models that could allow the prediction of the magnitude of the curvature. We found unexpected instability in dendritic-like vacancies and we suggest that the non-periodic character of the graphene quantum dot, in contrast to graphene, would prevent such vacancies to be relaxed in a higher extension, causing this kind of systems to be less stable than, for example, zigzag complementary figures systems.