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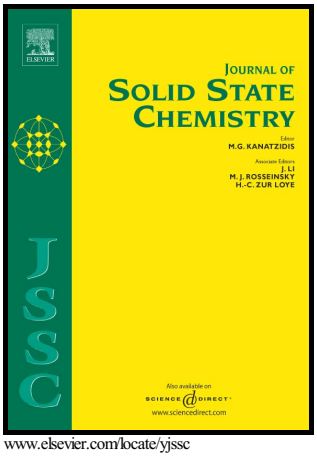

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Theoretical Study of Porous Surfaces Derived from Graphene and Boron Nitride

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Abstract

Porous graphene (PG), graphenylene (GP), inorganic graphenylene (IGP-BN), and porous boron nitride (PBN) single-layer have been studied via periodic density functional theory with a modified B3LYP functional and an all-electron Gaussian basis set. The structural, elastic, electronic, vibrational, and topological properties of the surfaces were investigated. The analysis showed that all porous structures had a nonzero band gap, and only PG exhibited a non-planar shape. All porous structures seem to be more susceptible to longitudinal deformation than their pristine counterparts, and GP exhibits a higher strength than graphene in the transversal direction. In addition, the electron densities of GP and IGP-BN are localized closer to the atoms, in contrast with PG and PBN, whose charge density is shifted towards the pore center; this property could find application in various fields, such as gas adsorption.

Graphical abstract

The structural, elastic, electronic, vibrational, and topological properties of the porous surfaces derived from graphene and hBN were investigated using DFT/B3LYP approach. The Raman fingerprints were obtained for the first time.