

Author's Accepted Manuscript

Theoretical Study of Porous Surfaces Derived from Graphene and Boron Nitride

G.S.L. Fabris, N.L. Marana, E. Longo, J.R. Sambrano



www.elsevier.com/locate/jssc

PII: S0022-4596(17)30433-4
DOI: <https://doi.org/10.1016/j.jssc.2017.10.025>
Reference: YJSSC19987

To appear in: *Journal of Solid State Chemistry*

Received date: 15 August 2017

Revised date: 11 October 2017

Accepted date: 18 October 2017

Cite this article as: G.S.L. Fabris, N.L. Marana, E. Longo and J.R. Sambrano, Theoretical Study of Porous Surfaces Derived from Graphene and Boron Nitride, *Journal of Solid State Chemistry*, <https://doi.org/10.1016/j.jssc.2017.10.025>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Theoretical Study of Porous Surfaces Derived from Graphene and Boron NitrideG. S. L. Fabris¹, N. L. Marana¹, E. Longo², J. R. Sambrano^{1*}¹Modeling and Molecular Simulation Group - CDMF, São Paulo State University, P.O. Box 17033-360, Bauru, SP, Brazil²Chemistry Institute - CDMF, Federal University of São Carlos, P.O. Box 14801-907, São Carlos, SP, Brazil

email: sambrano@fc.unesp.br

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.

Download English Version:

<https://daneshyari.com/en/article/7757872>

Download Persian Version:

<https://daneshyari.com/article/7757872>

[Daneshyari.com](https://daneshyari.com)