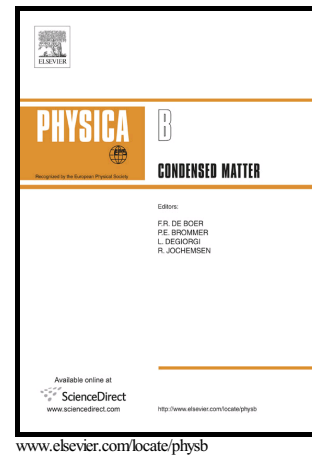


Author's Accepted Manuscript

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PII: S0921-4526(17)30405-2
DOI: <http://dx.doi.org/10.1016/j.physb.2017.07.016>
Reference: PHYSB310083

To appear in: *Physica B: Physics of Condensed Matter*

Received date: 25 January 2017
Revised date: 24 May 2017
Accepted date: 7 July 2017

Cite this article as: Julio C. Aguiar, Carlos R. Quevedo, José M. Gomez and Héctor O. Di Rocco, Theoretical Compton profile of diamond, boron nitride and carbon nitride, *Physica B: Physics of Condensed Matter* <http://dx.doi.org/10.1016/j.physb.2017.07.016>

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Theoretical Compton profile of diamond, boron nitride and carbon nitride

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Abstract

In the present study, we used the generalized gradient approximation method to determine the electron wave functions and theoretical Compton profiles of the following super-hard materials: diamond, boron nitride (*h*-BN), and carbon nitride in its two known phases: $\beta\text{C}_3\text{N}_4$ and $g\text{C}_3\text{N}_4$. In the case of diamond and *h*-BN, we compared our theoretical results with available experimental data. In addition, we used the Compton profile results to determine cohesive energies and found acceptable agreement with previous experiments.

Keywords: Compton profile; generalized gradient approximation; diamond; boron and carbon nitride

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