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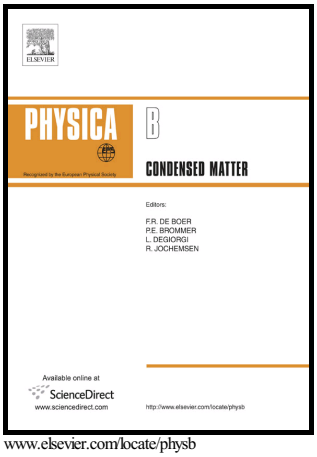

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Theoretical Compton profile of diamond, boron nitride and carbon nitride

Julio C. Aguiar[a,**]

[a] *Autoridad Regulatoria Nuclear, Av. Del Libertador 8250, (C1429BNP) Buenos Aires, Argentina.*

Carlos R. Quevedo[b*]

[b] *Universidad Nacional de Asunción, Facultad de Ciencias Exactas y Naturales (CC1039), Campus Universitario de San Lorenzo, Paraguay.*

José M. Gomez[b,c*]

[c] *Universidad Nacional de Asunción, Facultad Politécnica (CC2111), Campus Universitario de San Lorenzo, Paraguay.*

Héctor O. Di Rocco[d,e*]

[d] *Instituto de Física "Arroyo Seco", Facultad de Ciencias Exactas, Universidad Nacional del Centro de la Provincia de Buenos Aires, Pinto 399, (7000) Tandil, Argentina.*

[e] *Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina.*

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: βC_3N_4 and gC_3N_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

*Corresponding author
Email address: jaguiar@arn.gob.ar (Julio C. Aguiar[a,*])