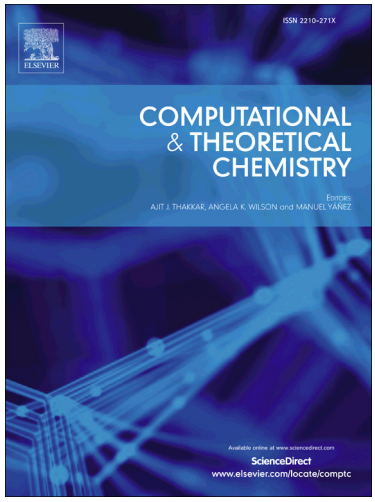

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Alexander M. Silva, Mariana I. Rojas

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Electric and Structural properties of Polymeric Graphite Carbon Nitride (g-C_3N_4): A Density Functional Theory study

Alexander M. Silva[1] *and Mariana I. Rojas*[2*]

[1]Divisão de Metrologia de Materiais, (INMETRO) Instituto Nacional de Metrologia, Normalizacão e Qualidade Industrial, Duque de Caxias, Río de Janeiro, RJ 25245-020, Brazil.

[2]INFIQC - Departamento de Matemática y Física, Facultad de Ciencias Químicas, Universidad Nacional de Córdoba – Ciudad Universitaria, 5000 Córdoba, Argentina.

KEYWORDS

Graphite carbon nitride; properties; Density Functional Theory calculation

ABSTRACT

Graphite carbon nitride (g-C_3N_4) is a new class of N-doped material that exists in 2D and 3D structures. They are nanoporous materials with multiple technological applications. That is why we present here a complete Density Functional Theory study about the properties of (2D) sheets: triazine and tri-s-triazine and the (3D) crystals. The layers can be stacked in different forms on the crystals. Thus, we consider different stacking types and calculate the adhesion energy