

## Accepted Manuscript

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PII: S2210-271X(16)30443-1

DOI: <http://dx.doi.org/10.1016/j.comptc.2016.11.004>

Reference: COMPTC 2290

To appear in: *Computational & Theoretical Chemistry*

Received Date: 19 September 2016

Revised Date: 14 October 2016

Accepted Date: 2 November 2016



Please cite this article as: A.M. Silva, M.I. Rojas, Electric and Structural properties of Polymeric Graphite Carbon Nitride (g-C<sub>3</sub>N<sub>4</sub>): A Density Functional Theory study, *Computational & Theoretical Chemistry* (2016), doi: <http://dx.doi.org/10.1016/j.comptc.2016.11.004>

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# Electric and Structural properties of Polymeric Graphite Carbon Nitride (g-C<sub>3</sub>N<sub>4</sub>): A Density Functional Theory study

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## KEYWORDS

Graphite carbon nitride; properties; Density Functional Theory calculation

## ABSTRACT

Graphite carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) 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

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