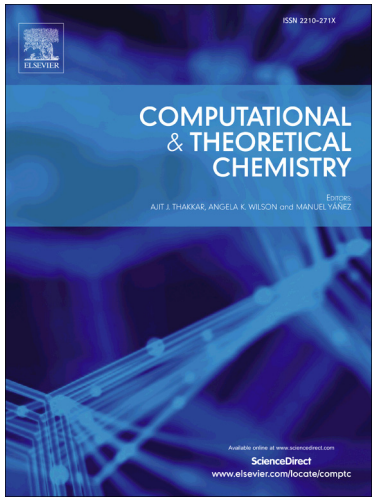

A DFT Study of the Electronic and Magnetic Properties of $C_{36}Si_{24}$ Fullerenes

F.G. Bernal Texca, E. Chigo-Anota, L. Tepech Carrillo, M. Castro

PII: S2210-271X(17)30020-8
DOI: http://dx.doi.org/10.1016/j.comptc.2017.01.013
Reference: COMPTC 2373

To appear in: *Computational & Theoretical Chemistry*

Received Date: 18 November 2016
Revised Date: 12 January 2017
Accepted Date: 13 January 2017

Please cite this article as: F.G. Bernal Texca, E. Chigo-Anota, L. Tepech Carrillo, M. Castro, A DFT Study of the Electronic and Magnetic Properties of $C_{36}Si_{24}$ Fullerenes, *Computational & Theoretical Chemistry* (2017), doi: http://dx.doi.org/10.1016/j.comptc.2017.01.013

A DFT Study of the Electronic and Magnetic Properties of $C_{36}Si_{24}$ Fullerenes

[1]F. G. Bernal Texca, [1,*] E. Chigo-Anota, [2]L. Tepech Carrillo, [3]M. Castro*

[1]*Benemérita Universidad Autónoma de Puebla, Facultad de Ingeniería Química, Ciudad Universitaria, San Manuel, Puebla, Código Postal 72570, México*.

[2] *Universidad Autónoma Benito Juárez de Oaxaca, Escuela de Ciencias, C.P. 68120, Oaxaca de Juárez, Oax. México*.

[3]*Universidad Nacional Autónoma de México-Departamento de Física y Química Teórica, DEPg-Facultad de Química, México D.F., C.P. 04510, México.*

Author to whom correspondence should be addressed; e-mail: [1,*] ernesto.chigo@correo.buap.mx
[3,*] miguel.castro.m@gmail.com

The structural stability, electronic and magnetic properties of a new silicon carbide fullerene, of chemical composition $C_{36}Si_{24}$ (SiCF), rich in carbon atoms, were analyzed by means of density functional theory. Calculations were done using a exchange–correlation functional developed by Heyd-Scuseria-Ernzerhof, within the generalized gradient approximation (HSEh1PBE-GGA), and 6-31G(d) basis sets of Pople *et al*. The DFT simulation results reveal structural stability for the $C_{36}Si_{24}$ system, which, in a neutral charge state, behaves as semiconductor non-magnetic nanomaterial, since the HOMO-LUMO gap is 0.89 eV. The SiCF system shows marked polarity (1.16 D) and low chemical reactivity. Interestingly, the properties of the silicon carbide fullerene evolve in such way that a semiconducting non-magnetic to conducting magnetic transition is observed for the case where small quantities of nitrogen atoms act as substitutional impurities ($C_{36-X}Si_{24}N_X$; X=1,2,5, and 10). This electronic behavior was reached for x = 1 and 5 dopes, yielding magnetic moments of 1.0 magneton bohr (μ_B). Additionally, low work function occurs on this CSiN fullerene, which is crucial for the design of electronic devices.

Keywords: $C_{36}Si_{24}$ fullerene; Electronic Properties; Magnetic Properties; Work function; DFT theory