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

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A DFT Study of the Electronic and Magnetic Properties of C₃₆Si₂₄ Fullerenes

¹F. G. Bernal Texca, ^{1,*}E. Chigo-Anota, ²L. Tepech Carrillo, ³M. 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 C₃₆Si₂₄ (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 C₃₆Si₂₄ 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}Si₂₄N_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: C₃₆Si₂₄ fullerene; Electronic Properties; Magnetic Properties; Work function; DFT theory

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