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ORIGINAL ARTICLE

Adsorption of Metronidazole drug on the surface of nano fullerene C_{60} doped with Si, B and Al: A DFT study

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Abstract

In this research, the quantum mechanics calculations were carried out to elucidate the adsorption behavior of metronidazole drug on the surface of pristine as well as doped C60 fullerene with Si, B and Al using density functional theory (DFT) at B3LYP/6-31G (d,p) level. After optimization of the structures, various parameters such as HOMO and LUMO energies, gap energy, adsorption energy, chemical hardness, chemical potential, dipole moment, electrophilicity index and thermodynamics data were calculated. The results showed that by substitution of the carbon atom in the C60 fullerene with Si, B and Al, the amounts of gap energy and chemical hardness are decreased, while those of chemical potential and electrophilicity index are increased. It means that the doping of C60 by Si, B and Al leads to an increase in drug reactivity. Also, the binding and stabilization energies are increased by doping of C60. The thermodynamic results suggested that substitution on the pristine C60 leads to a more negative in the value of the Gibbs energy and subsequent spontaneous process.

Keywords: *Chemical Potential; C60 Fullerene; Density Functional Theory (DFT); Doping; Metronidazole.*

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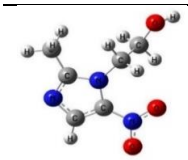
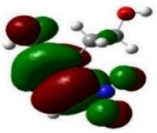
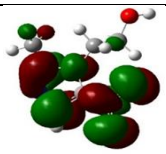
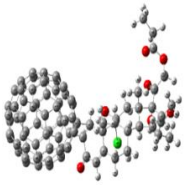
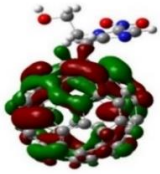
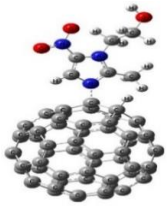
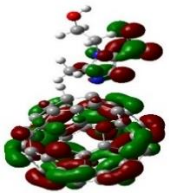
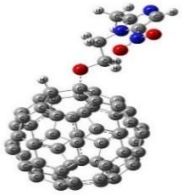
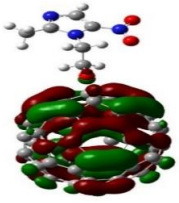
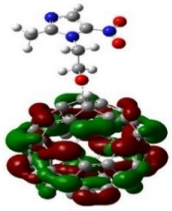
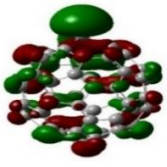
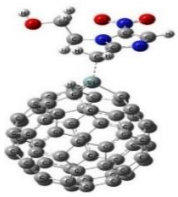
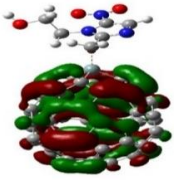
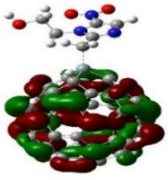
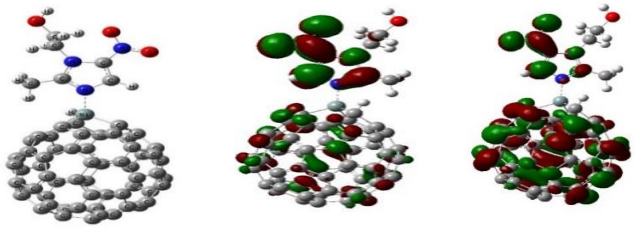
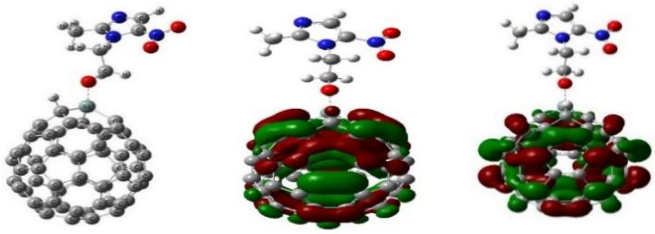
Adsorption of Metronidazole drug on the surface of nano fullerene C_{60} doped with Si, B and Al: DFT Study

	Optimal Structures	HOMO orbitals	LUMO orbitals
Metronidazole			
C_{60}			
C_{60}-C-Met			
C_{60}-N- Met			
C_{60}-O- Met			
C_{59}Si			
C_{59}Si-C- Met			

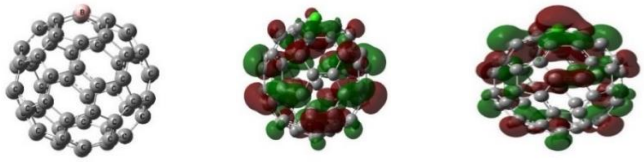
C_{59}Si-N- Met



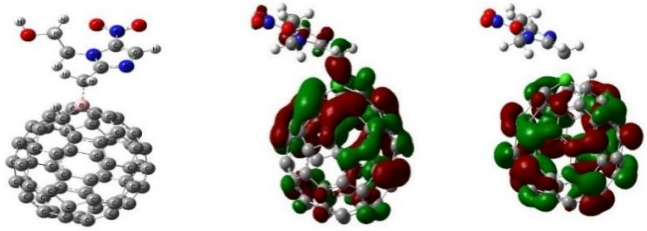
C_{59}Si-O- Met



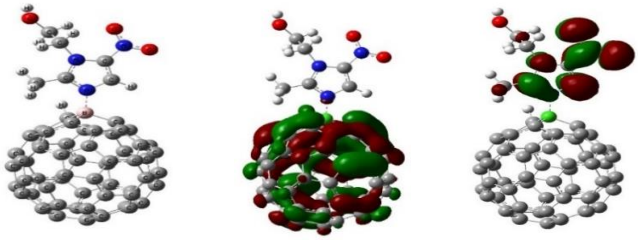
C_{59}B



C_{59}B-C- Met



C_{59}B-N- Met



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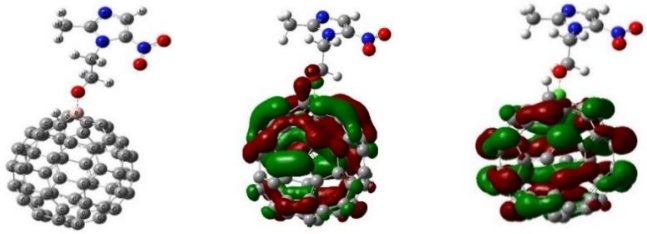
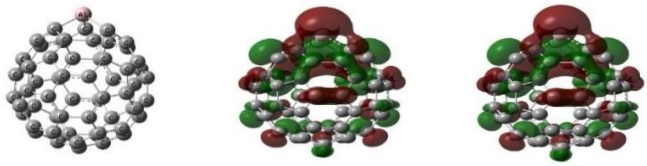
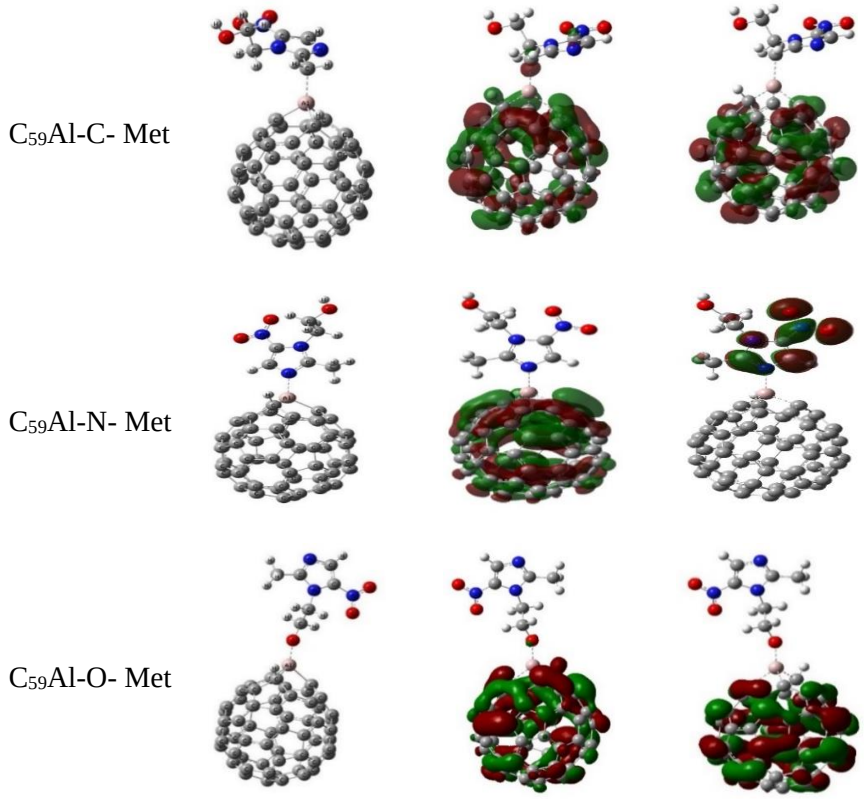


C_{59}Al





S-1. Schematic of HOMO/ LUMO orbitals of drugs and drug-nanocarriers.