

A DFT study of the binding of aryl and alkyl radicals to the B12N12 nanocage cluster

Avni Berisha

University of Prishtina "Hasan Prishtina", Prishtina, Republic of Kosovo

avni.berisha@uni-pr.edu

The interaction, electronic and optical properties of octahedral B12N12 nanocage cluster covalently modified from the attachment of alkyl and aryl radicals¹ were analyzed using Density Functional Theory calculations. At $T = 298.15$ K in the vacuum and solvent, the measured adsorption and binding energies of aryl (Figure 1) and alkyl radicals with the B12N12 fullerene are also evaluated. In order to classify the most significant changes occurring as a result of interactions between B12N12 fullerene and radicals, UV absorption and IR spectra were computed and analyzed.

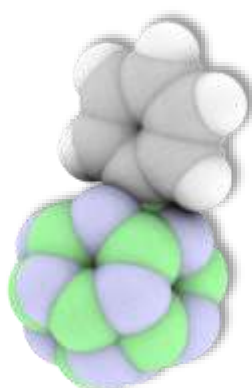


Figure 1. The optimized geometry of grafted B12N12 nanocage cluster by a phenyl group.

The adsorption of the aryl or alkyl diazoniums onto the B12N12 surface, where van Der Waals interactions play a major role, is a first step prior to grafting reaction. Furthermore, the transition state indicates that the interaction of aryl and alkyl radicals indicates that the modification steps is spontaneous.

References

- [1] Berisha, A., Chehimi, M. M., Pinson, J. & Podvorica, F. I. Electrode Surface Modification Using Diazonium Salts. in *Electroanalytical Chemistry* 115–224 (CRC Press, 2015).