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Investigation of the interaction of boron nitride nanosheets (h-BN) with cyanogen fluoride (FCN) by density functional theory method

M. Talaei, A. Bagheri, M. Abasi, M. Siahvoshi, M. Rezaei Sameti*
Department of Applied Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran
E-mail: mrsameti@malayeru.ac.ir

Abstract

Among various nanomaterials, carbon-based nanostructures are one of the major types of DDC, utilized in various configurations like nanoparticle, nanotube, graphene and graphene oxide [1–3].The aim of this work was to investigate the adsorption and detection of cyanogen fluoride (FCN) molecule on a boron nitride nanosheet marked with hydrogen ion (H^+) in the presence and absence of an electric field. Calculations were performed using density function theory (DFT/WB97XD) and 6-31G(d,p) base set by Gaussian 16 software. After calculations, quantum and thermodynamic parameters, absorption energy, UV spectra, HOMO and LUMO orbitals, DOS and RDG diagrams, optical properties and other results were extracted. The values of enthalpy and adsorption energy are negative for all absorption models, indicating that the adsorption process is exothermic in all models. Gibbs free energy is negative in most absorption models, which indicates that the adsorption process is spontaneous in these models. The results of AIM, RDG and NBO show that the adsorption of cyanogen fluoride on the boron nitride nanosheet is hydrogen and van der Waals type. Applying an electric field and adding hydrogen ions to the nanosheet reduces the absorption energy, gap energy and hardness of the nanosheet, which can lead to stronger adsorption, increased conductivity and reactivity of the nanosheet. These results suggest that boron nitride marked with hydrogen ions in the presence of an electric field can be a good choice for the adsorption and detection of cyanogen fluoride.

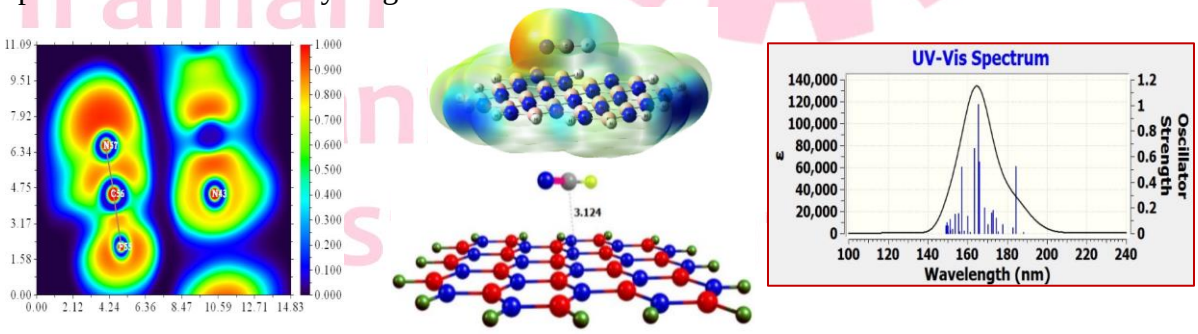


Figure 1 : The ELE , MEP, UV-visible and optimized sturctures of FCN@h-BN nano sheet

Keywords: *h*-BNanosheet, Cyanogen Fluoride, Hydrogen Ion, Electric Field, DFT

References

[1] M. Solimannejad, R. Rahimi, S. Kamalinahad, *J. Inorg. Organomet. Polym Mat*. **2017,** *27*, 1234.
[2] M. Rezaei‑Sameti, P. Zarei, P. *Adsorption.* **2018,** 24, 757.
[3] M. Doust Mohammadi, H. Y. Abdullah, *J. Comp. Biophy. Chem*. **2021,** 20, 765.