**Computer modeling of the interaction process of the fullerene C60 molecule with the surface of an aluminum substrate**

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In this research work, the adsorption of fullerene C60 molecule on aluminum Al(001) surface was simulated in the open source LAMMPS package based on the Molecular dynamics method. The results were obtained by expressing the Al-Al, C-C and Al-C interactions between the aluminum substrate and the atoms constituting the fullerene molecule using the second-order interatomic potential Tersoff potential [1]. The aluminum substrate on which the adsorption of fullerene C60 molecule was observed consists of a cubic single crystal with a size of 18.34×18.34×18.34 Å and has 500 atoms. The adsorption process was carried out at a temperature of 0 K, and to ensure the stability of this temperature, a Noza-Hoover [2] thermostat was used in the NVT ensemble. The adsorption energy of the fullerene molecule on the substrate surface was determined by energy minimization.



Figure 1 a) Fullerene molecule adsorbed on the (001) surface of the substrate.

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The results obtained show that the adsorption of the fullerene C60 molecule with a pentagonal configuration on the substrate surface is stable and consists of chemical adsorption with an energy of E ads = 3.10 eV. It was also found that the average length of the Al-C bonds formed during this interaction is equal to λ = 2.46 Å.

[1] G. Plummer and G.J. Tucker, Physical review B, Vol. 100, pp. 214114, 2019.

[2] Hoover, W.G., “Canonical dynamics: Equilibrium phase-space distributions”, Physical Review A, Vol. 31, 1695, 1985.