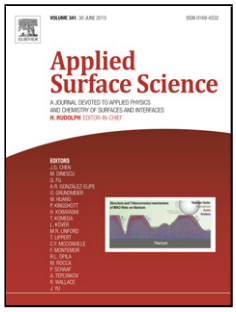

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An investigation of the adsorption of potassium stearate molecules on diamond-like carbon substrate using molecular dynamics simulation

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Highlights

- The adsorption of potassium stearate molecules on diamond-like carbon substrate was studied using MD simulation.
- Strong attractive interactions between cluster molecules will prevent the adsorption significantly.
- Confinement conditions imposed on molecular clusters will promote the adsorption of molecules.
- Polar end groups tend to accumulate and construct a steady chain structures after reaching equilibrium.
- Changes in the inter- and intra-subsystem potential with and without confinement conditions was investigated.

Abstract Molecular dynamics (MD) simulations were performed to investigate the adsorption of potassium stearate molecules on diamond-like carbon (DLC) substrate. The effects of non-bonded interactions and confinement conditions on the adsorption were investigated. The confinement conditions performed herein were achieved by imposing a Z-direction constraint on the movement of molecules in the initial stage of adsorption, and then releasing the molecules from the constraint gradually. Our simulation results show that the polar end groups of molecules tended to accumulate during the adsorption, and the final distribution of adsorptive film without confinement was irregular. Under confinement conditions, the adsorptive film was evenly distributed on the substrate after reaching its equilibrium configuration, and the final inter-subsystem potential of the substrate on adsorptive film was obviously decreased as compared with the results without confinement. These findings provided an effective approach for promoting the adsorption of molecules.

Keywords: potassium stearate; diamond-like carbon; molecular adsorption; non-bonded