Molecular investigation of water adsorption on graphene and graphyne surfaces

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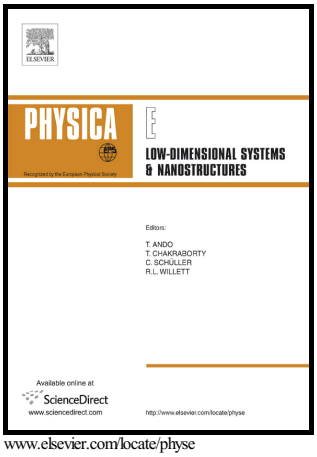

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Abstract

In this paperthe adsorption action of a water droplet on the graphene and graphyne externals has been examined. Conclusions received from the calculation of the water contact angle on the graphene and the graphynes surfaces have demonstrated that graphyne is more hydrophobic than graphene. Sketching the contour maps of the water interaction showed different behaviors of water droplet on these surfaces. The results show that water molecules, form a sub_layer of water on the graphyne substrate while this sub_layer does not exist on the graphene. Molecular investigations of the water on the surfaces show that the attendance of a sub_layer of water on the substrate can cause changes in the structural properties of water droplet,changes such as the number of hydrogen bonds per water molecule in the water droplet, the order of molecules in different layersof water droplet and forces parallel to the surface between surface water molecules and substrate. In this study it was investigated that the interaction between the waters in the sub_layer and the waters in the first layer of water droplet close to the substrate can affect the behavior of water near the substrate.

Keywords:

Nano Water Droplet; Graphyne; Graphene; Wettability; Molecular Dynamic Simulation.