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Molecular dynamic study on graphene-based chemical sensors: adsorption studies and substrate effect

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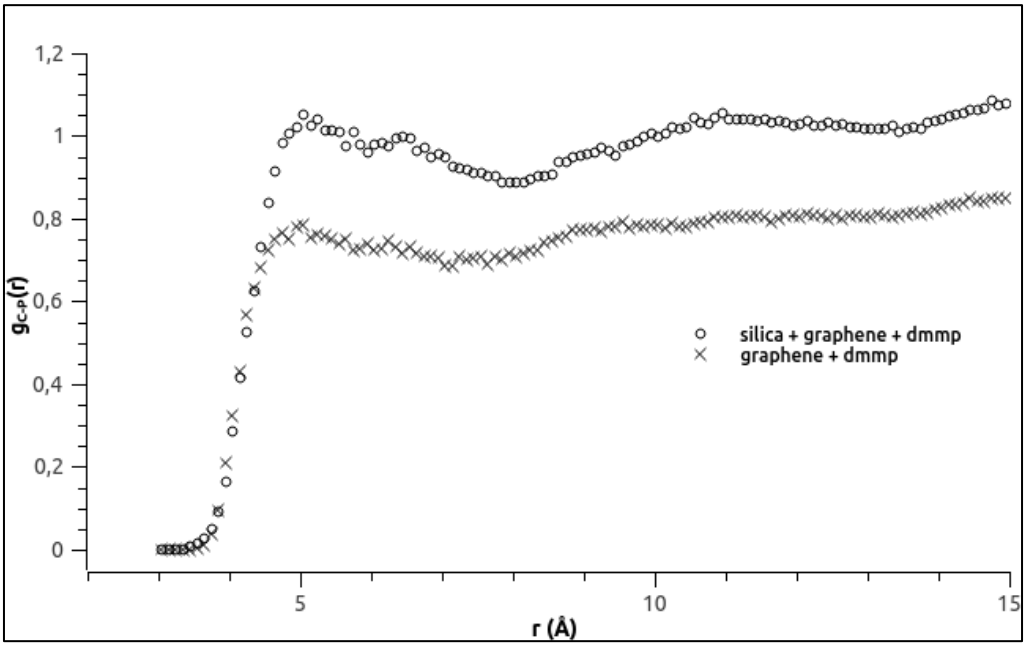
The monitoring and control of gas concentration have an essential role in several technological areas [1-3]. In this context, graphene-based materials have been considered interesting candidates for applications in chemical sensors. Besides of presenting unique electrical, mechanical and structural properties, these compounds have also shown high sensitivity for the detection of toxic gases [4-6]. However, some recent studies suggest that the sensory properties of graphene are not intrinsic, but they are associated with the presence of defects in the substrate on which it is deposited [7], suggesting that electrostatic graphene/substrate interactions may be relevant for the formation of adsorption centers. In this context, in the present work we carried out a series of adsorption studies of dimethyl methylphosphonate (DMMP) molecules on the surface of graphene nanosheets in the presence of a silica substrate. The simulations were carried out via molecular dynamic calculations (MD) considering systems composed of a two dimensional graphene nanosheet, 1000 DMMP molecules and a silica substrate. Classical force fields were employed to the system and NPT and NVT ensembles were considered at 300 K and 1.0 atm, considering a 90 A x 90 A x 90 A simulation box. The calculations were implemented with the aid of LAMMPS computational package [8]. As shown in Figure 1 the results indicate that the presence of silica substrate intensify the interaction between the graphene nanosheet and the analyte (DMMP), suggesting that specific interactions between the nanosheets and the substrate are indeed relevant to improve the sensory properties of graphene.

***Figure 1**. Radial distribution function for the carbono(C) belonging to graphene and phosphorus and the phosphorus (P) of the DMMP molecule.*



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