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PS3-21 Interaction of lons with Graphene on a Substrate

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In this paper analyzes the process of dynamic screening of external charges, moving over the surface of graphene disposed on a substrate. We are considered here relatively slow ions with velocities from thermal speeds to Bohr velocity. We explore here the effects of dynamic polarization of graphene on a substrate by ion motion parallel to its surface. We limited the study of the effects associated with the presence of an insulating substrate, such as , with a dielectric constant of . Ishigami et al. [1] have found that the distance h between graphene and substrate is on the order of the distance between graphene layers in graphite or even larger. Only (according to our information) in the paper [2] considered the effects of finite h. Our principal goal was to demonstrate how strong are the effects of finite h on the degree of dynamic polarization of graphene moving ions. This meant the need to include the gap size graphene-substrate as a parameter in modeling phenomena screening graphene. The simulation was performed by molecular dynamics using ReaxFF potential of free package for classical molecular dynamics LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator).

References

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