Electronic transport properties of graphene in different aqueous solutions

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Graphene has the potential to induce significant change in the way we construct and use electronic devices. However, on the one hand, the presence of water molecules – even at low concentrations – is unavoidable, and such effects on the electronic transport properties could be significant. On the other hand, many possible applications include biological systems or molecules. In those cases, the device unavoidably is embedded in an aqueous solution. The effects of this solution is not fully known, and from a computational point of view, is quite challenging.

The methodology known as QM/MM is very useful for modeling large systems as realistically as possible as it separates a particular system into two subsystems treated at different levels of theory. In our case, a periodic simulation box with graphene, water molecules and counter-ions (NaCl) sampled via Molecular Dynamics can be divided into a classical and a quantum part. The solvent can be treated by molecular mechanics methods while the graphene sheet must be treated quantum mechanically (via density functional theory), since we want to investigate the electronic transport throughout the sheet. Finally, the electronic transport properties are obtained via the non-equilibrium Greens functions formalism.

Thus, in this work we will present an extensive investigation of the electronic transport properties of solvated graphene using this technique. We performed simulations of graphene in different solvation conditions by varying the concentration of NaCl. We also tested the rigid rod model for polarization in graphene, as implemented in GRAPPA [1] force field, in order to improve the description of the liquid-graphene interactions. Our results show that the electronic transport properties of solvated graphene are extremely sensitive to the presence of a solvent but not very sensitive to a salt, even in high concentration in the solution. The overall trend for the presence of water is to induce a chemical gating effect that shifts the local Fermi level of graphene, leading to doping of the sheet.