Selective adsorption behavior of mixture solutions on functionalized graphene

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Filtration is very much important technology especially in the separation field. To study filtering solvent, one must understand core mechanism, which resides in the intermolecular interactions between solvent and surface. In this study, we introduce three types of surfaces, which are nickel, pristine graphene, and HDFS (heptadecafluoro-1,1,2,2,-tetrahydrodecyl-trichlorosilane)-functionalized graphene, to capture adsorption properties of solutions, which are chosen to be water, gasoline, kerosene and olive oil. Thereafter, correlation of adsorption property to selective filtration is established via simple force balance formulated by adhesive force between solvent and surface, surface tension of solvent, and the gravitational force. The adhesive force was obtained from constant-temperature molecular dynamics (MD) simulation and the surface tension was calculated based on surface physics in consideration of simplified morphology of the substrate. Particularly, from this study, we were able to anticipate selective filtration of solvents by substrates with different surfaces.