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Liquid Separation by a Graphene Membrane[1] GUSTAVO DALPIAN, EUDES FILETI, Universidade Federal do ABC, Brazil, ROBERTO RIVELINO, Universidade Federal da Bahia, Brazil — The behavior of liquids separated by a one atom thick membrane (graphene) is studied by using extensive molecular dynamics (MD) simulations at different conditions. With the help of appropriate empirical potentials, we investigate two liquid phases forming distinct systems: XGY, where X represents water or benzene, G represents a graphene sheet, and Y represents water, benzene or acetonitrile. Our MD simulations reveal important changes in the wettability patterns of these liquids near graphene. For instance, water-graphene-water exhibits strong density oscillations in a thin interfacial region of 2.3 nm. In the cases of separate benzene and/or acetonitrile the oscillating-density interfacial region extends beyond 3 nm, under similar thermodynamic conditions. Interestingly, our findings indicate that a liquid in one side of the membrane can affect the degree of wetting on the other side. Also, we show that high pressure effects, up to 10 kbar, can lead liquid water to be highly ordered along the normal direction of the graphene sheet.

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