

Hydrophilic and hydrophobic interactions: from materials to living cells

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I will discuss simulations where chemical interactions are coarse grained to the level of hydrophilic and lipophilic interactions. At the nanometric level, I will examine the interactions of lipid bilayers with variously functionalized graphenes and discuss the results in terms of nanotoxicology. At the micrometric level, I will show that the mechanical response of living cells on a 2D pattern of chemical cues can be modelled. The cells are effectively represented by drops that are endowed with the presence of additional forces that make them active. With the proper choice of these forces, the phenomena that emerge from the dynamics simulations match the experiments. In particular, a combination of hydrophilic and lipophilic forces allows the active drops to respond to geometric shape cues and form squares, pentagons, hexagons and flowers, just as living cells do. The mechano-chemical interactions that orchestrate cell behavior are therefore harnessed and used to beat the surface tension that characterizes an inactive drop.