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# 42 - Adsorption of organic molecules on solid surfaces using surfactants: A Molecular dynamics study

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Using simulations of Molecular Dynamics, we investigated the role of surfactant molecules to be used as agents to capture molecules on solid surfaces, either to remove alkane molecules from a graphite surface or to absorb CO2 in a zeolite. Removal of alkanes from graphite plates simulations on three different surfactants, Cocamidopropyl betaine (CAPB), N-dodecyl-N.N-dimethyl-3-ammonio-1-propane-sulfonate (SB3-12), Sodium dodecyl sulfate (SDS), and their mixtures at different compositions were carried out. The study was conducted with different concentrations of decane on the surface and in all cases the alkane molecules were adsorbed on the solid surface in a layer structure, two or three layers, suggested by the density profiles. Surfactants promoted the formation of an additional decane layer, indicating gas separation or removal from the graphite surface. It is shown that mixtures seem to be the best way to remove the alkanes from the surface. Studies of CO2 capture in a zeolite structure were also conducted with and without SDS surfactants on the solid surface. A new force field for CO2 was proposed which reproduced better some thermodynamic properties. Simulations at different SDS and CO2 concentrations were carried out and it was observed that the best gas adsorption occurs for low CO2 concentration with a few surfactants on the surface. Moreover adsorption was mainly conducted from the free ions in the zeolite as indicated by the pair correlation functions.
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**Authors:** Prof. DOMINGUEZ, Hector (National Autonomous University of Mexico); Ms SALAZAR-ARRIAGA, Ana (National Autonomous University of Mexico); Ms VALENCIA-ORTEGA, Minerva (National Autonomous University of Mexico); Dr FUENTES-AZCATL, Raul (National Autonomous University of Mexico)

**Presenter:** Prof. DOMINGUEZ, Hector (National Autonomous University of Mexico)

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