Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular Dynamics study of $CaCO_3$ nanoparticles in hydrophobic solvent with stearate co-surfactant: Supporting Information

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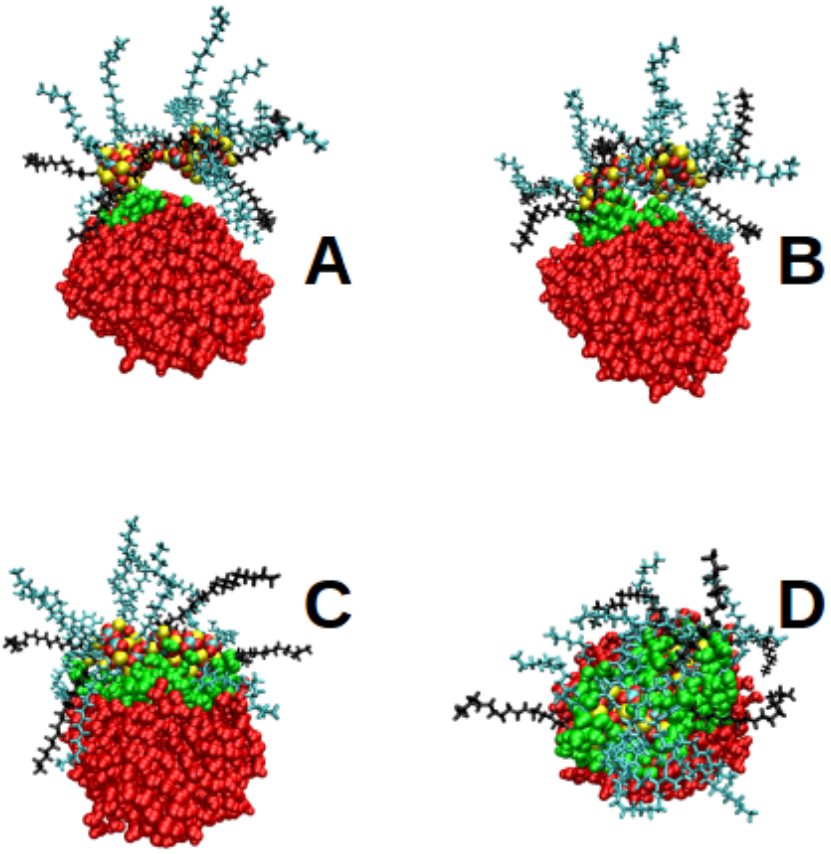

Figure 1: MD snapshots during a 20 ns simulation of a salicylate/stearate nanoparticle and a representative water droplet, showing the successive stages of a) initial bridge formation, b) bridge development, c) water coating of the nanoparticle, and d) full nanoparticle adsorption into the water drop. Water molecules within 7 Å of the nanoparticle are shown as green spheres, with rest represented by red spheres. Calcium ions are shown in yellow. The cyan and red spheres represent the carbon and oxygen atoms, respectively of the carbonate ions. The salicylate surfactants are shown in cyan, with the stearate co-surfactant shown in black.