Modelling of Pickering emulsion stabilization

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The formation of Pickering emulsions was investigated by Langevin dynamics method. The kinetics of SiO_2 nanoparticle adsorption on the surface of oil droplets and the structure of adsorbed layer was analyzed. Calculations were performed by using physical and chemical parameters obtained in laboratory experiments or reference data.

The influence of nanoparticle and droplet parameters on emulsion stability was numerically determined. Emulsion stability diagram was obtained that presented the regions with emulsions unstable and stable towards flocculation and coalescence.

Highly ordered nanoparticle layer with a high level of surface coverage was observed in emulsions stable to flocculation and coalescence (Figure 1a). In the case of low velocity of nanoparticle adsorption tenuous layer was formed (Figure 1b) that accomplished by droplet flocculation. Local domains with ordered hexagonal structures were found in the systems with nanoparticle amount not enough to cover the surface of oil droplets and at high salt concentration in aqueous phase (Figure 1c). In spite of low surface coverage the flocculation was not observed in these emulsions for a long time. Silica nanoparticles formed extended and ramified aggregates at high ionic strengths of aqueous phase and large amounts of nanoparticles. Such aggregates formed the network that separated oil droplets and prevented their coalescence (Figure 1d).

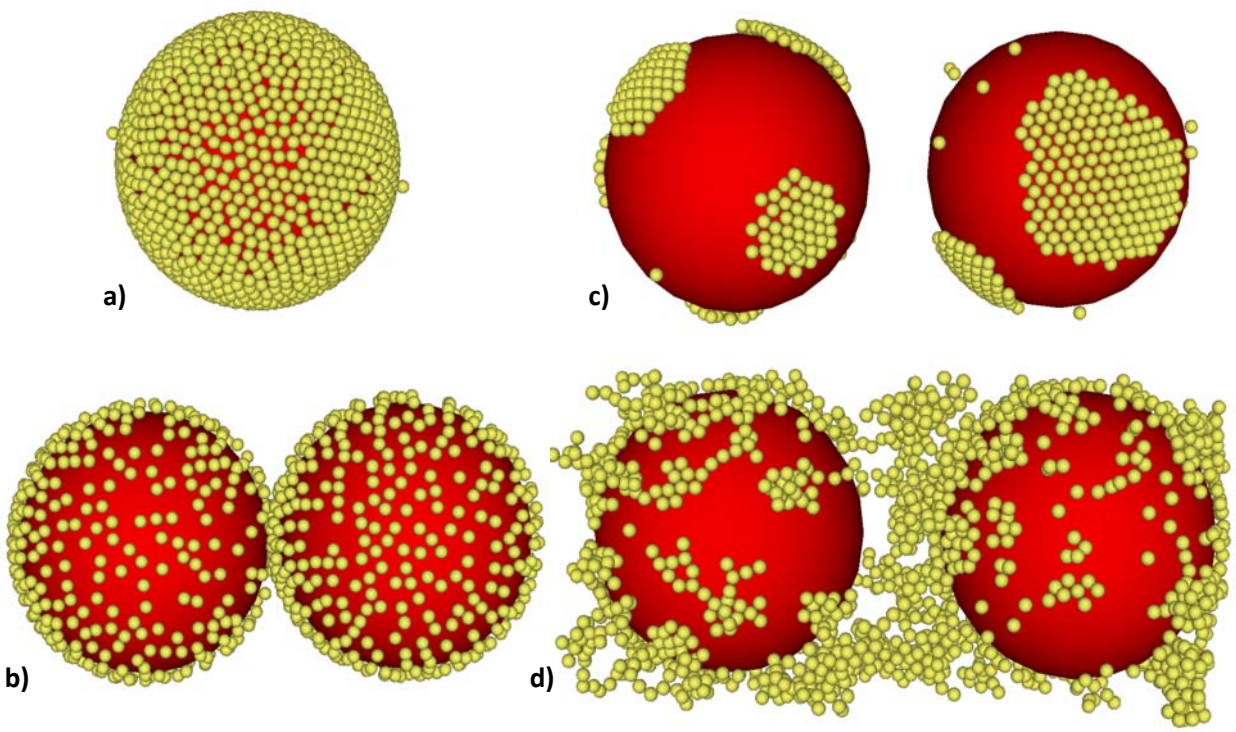

Figure 1 Snapshots of oil droplets with SiO_2 nanoparticles at ionic strength (I) 50 mM and nanoparticle number (N) 1500 (a), I = 10 mM, N = 1000 (b), I = 1000 mM, N = 250 (c), I = 2000 mM, N = 2000 (d).

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