Solubility and transport of cationic and anionic patterned nanoparticles

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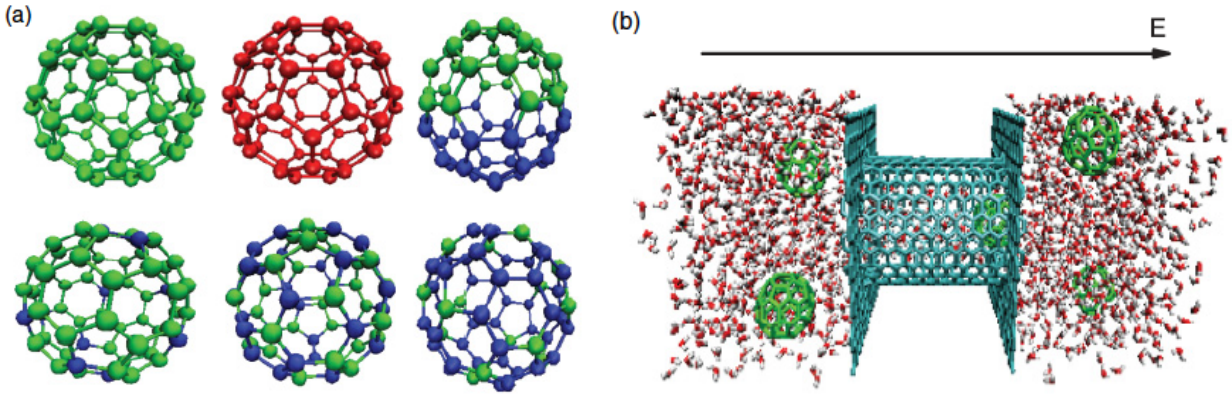
We analyze bulk diffusion and transport through hydrophobic nanochannels of nanoparticles (NPs) with different hydrophobic-hydrophilic patterns achieved by coating a fraction of the NP sites with positive or negative charges via explicit solvent molecular dynamics simulations. Ten different charge pattern types including Janus charged-hydrophobic NPs are studied.

- The cationic NPs are more affected by the patterns and have higher diffusion constants and fluxes than their anionic NPs counterparts. The NP-water interaction dependence on surface pattern and field strength explains these observations.
- The NP-water Coulomb interaction of anionic NPs in the bulk, which are much stronger than the hydrophobic NP-water interactions, are stronger for NPs with higher localized charge, and stronger than in the cationic NPs counterparts.
- The diffusion and transport of anionic NPs such as proteins and protein charge ladders with the same total charge but different surface charge patterns are slowest for the highest localized charge pattern, which also adsorb strongest onto surfaces.

Our model demonstrates the separation (by reverse osmosis, capillary electrophoresis, or chromatography) of cationic NPs, including proteins with equal net charge but different surface charge distributions.



(a) Nanoparticle types: All have ±6e total charge. Green and red represent positive and negative charges, respectively, while blue denotes neutral, and (b) a snapshot of MD simulation system.

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