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Solubility and transport of cationic and anionic patterned nanoparticles JIAYE SU, HONGXIA GUO, Beijing National Laboratory for Molecular Sciences, Joint Laboratory of Polymer Sciences and Materials, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University — Diffusion and transport of nanoparticles (NPs) though nanochannels is important for desalination, drug delivery, and biomedicine. Their surface composition dictate their efficiency separating them by reverse osmosis, delivering into into cells, as well as their toxicity. We analyze bulk diffusion and transport through nanochannels of 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. The cationic NPs are more affected by the patterns, less water soluble, 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. For equivalent patterns, anionic NPs solubilize more than cationic NPs since the Coulomb interaction of free anionic NPs, which are much stronger than hydrophobic NP-water interactions, are about twice that of cationic NPs.

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