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Gas Transport in Polymer-Grafted Nanoparticles KAI ZHANG, SANAT KUMAR, Columbia University — The efficient separation of gases is crucial for clean energy technologies. With their intrinsic multiscale features and excellent self-assembly properties, polymer-grafted nanoparticles (PGNP) material makes a good candidate for effective gas separation, but the basic understanding of gas transport in PGNPs is still missing. While the nanoparticles cores are spherical, the corona of the PGNPs can be deformed into anisotropic space-filling polygons at high density that are commensurate with the crystal structures (Wigner-Seitz cells). Such deformation indicates that the polymer chains are extended or compressed along different directions and create cavities within the crystals that can help to improve the gas selectivity. We use coarse-grained computer simulations to study the solubility and diffusion of gas molecules inside the crystalline packing of the NP cores. By tuning the degree of polymerization, the surface density of grafting chains and the size of gas molecules, we systematically investigate the dependence of gas transport on these parameters. We find that the void formed by three contacting monomers imposes a critical lengthscale beyond which the transport becomes highly size selective.

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