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Diffusion and Filtration Properties of Self-assembled Close-packed Nanocrystal Membranes JINBO HE, The University of Chicago, XIAO-MIN LIN, Argonne National Laboratory, LELA VUKOVIC, HENRY CHAN, PETR KRAL, University of Illinois at Chicago, HEINRICH JAEGER, The University of Chicago — Small dyes are known to be able to penetrate through randomly packed nanoparticle monolayers, but a detailed understanding of the mechanisms for transport through the interstices between nanoparticles is still lacking. We report on systematic measurements of molecular transport across monolayers of close- packed, 5 nm diameter gold nanocrystals ligated with dodecanethiol. For water we find a filtration coefficient two orders of magnitude larger than for polymer-based nanofiltration membranes, while the self-diffusion coefficient is more than 100x smaller than in films of pure hydrocarbons. As we confirm by molecular dynamics simulations, larger molecules (tested molecular weight range: 200 - 43000) are unable to diffuse through the ligands. Instead, they most likely move through nm-sized regions of reduced ligand density, which are formed by slight variations in the local packing configuration and orientation of neighboring nanocrystals. In this intermediate size range we also find a pronounced dependence of the rejection rate on the molecules' charge. Molecules with cross-section above 2 nm are totally rejected.

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