

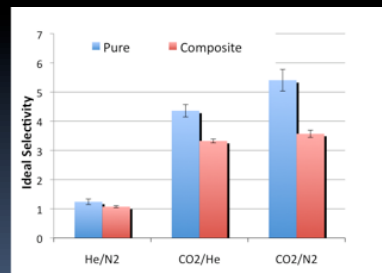
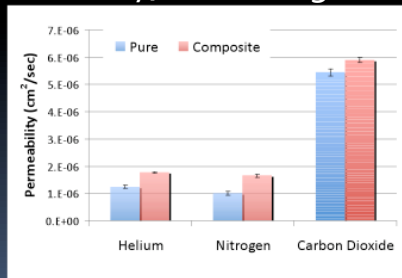
Tuning Small-Molecule Permeability in Polymeric Membranes with Nanoparticles

Nancy K. Lape, Department of Engineering, Harvey Mudd College, Claremont, CA 91711

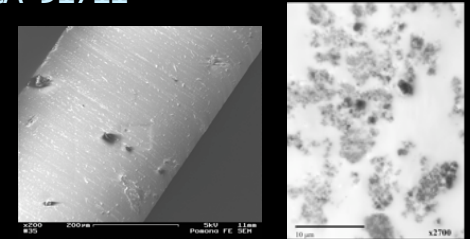
Background: To efficiently and effectively separate gas mixtures, membranes must exhibit both high gas permeability (fast transport) and high selectivity for one gas over the other. Unfortunately, these properties tend to be diametrically opposed: membranes made of rubbery polymers have high permeabilities but low selectivities, while membranes made of glassy polymers have high selectivities but low permeabilities. It has long been accepted that the addition of micron-sized inert impermeable particles to a polymer film decreases the permeability while leaving the selectivity unchanged. However, recent research has shown that adding nanoparticles to a special class of glassy polymers results in an *increase* in permeability, while retaining or possibly even improving the selectivity.

Our Work: We are examining the crossover between permeability enhancement and reduction with changes in particle size and polymer type.

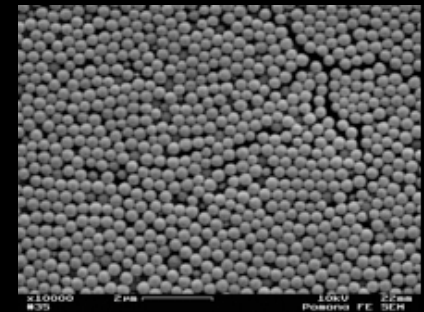
- Experimental: We have cast poly(dimethyl siloxane) (PDMS) and PDMS/silica composite films and synthesized silica particles of various sizes using the Stober process. Gas permeation experiments on the pure and composite membranes showed an increase in permeability upon addition of silica nanoparticles, but a simultaneous decrease in selectivity, indicating the presence of non-selective voids.



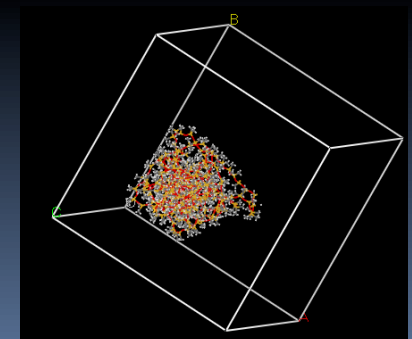
- Modeling: We modeled gas permeation in PDMS using Accelrys' Materials Studio and found... We plan to examine the change in free volume upon particle addition and the polymer-particle interface for PDMS and then extend to standard glassy polymers and ultra-high free volume glassy polymers.



SEM (left) and TEM (right) micrographs of cross section of PDMS/10 wt % 3-nm SiOx membrane.



SEM micrograph of SiOx particles synthesized via the Stober process.



Molecular Dynamics screenshot containing unit cell with a non-equilibrated PDMS chain.