Molecular dynamics simulations of nanoconfined solvents *(Prof. Ward H. Thompson).* Nanometer-sized cavities and pores can now be routinely generated in sol-gels, reverse micelles, zeolites, and even proteins, giving strong impetus to improving our understanding of chemistry in confined solvents. These cavities can serve as "nanoreactors" in which a chemical reaction takes place in the small pool of solvent allowed in this restricted space. However, little is known about how the confining framework properties affect chemistry in the confined solvent. In one project, an REU student will carry out molecular dynamics simulations of acetonitrile confined in nanoscale silica pores (using previously developed model pores). These simulations will allow the student to determine the structure of the nanoconfined acetonitrile liquid as well as the diffusive and reorientational properties. Further, the student will also investigate the effect of pore radius and surface chemistry (*e.g.*, by changing the pore termination from –OH to $–O(CH_3)_3$). These results will provide important comparisons to experimental results and have implications for the design of mesoporous catalysts. Since arriving at KU in 2001, Prof. Thompson has published or submitted three papers with undergraduate authors including two with REU students. Prof. Thompson routinely collaborates and publishes with synthetic organic and inorganic colleagues.

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