West Virginia University

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Multi-Scale Modeling of Aqueous Phase Methane Diffusion in Silicate Frameworks

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Silica-based materials including zeolites are commonly used for wide ranging applications including separations and catalysis. Substrate transport rates in these materials often determine the efficiency of such applications. Two factors that contribute to transport rates include 1) the porosity of the silicate matrix and 2) non-bonding interactions between the diffusion species and the silicate surface. Here, we utilize computer simulation to resolve the relative contribution of these factors to effective methane transport rates in prototypical silicate frameworks. Specifically, we are developing a 'homogenized' model of methane transport valid at micron and longer length scales that incorporates atomistic-scale kinetic information. The atomistic-scale data are obtained from extensive molecular dynamics simulations that yield local diffusion coefficients and potentials of mean force. With this model, we demonstrate how nuances in silicate hydration and silica/methane interactions impact 'macroscale' methane diffusion rates in bulk silicate materials.

Date: Wed, Dec. 5, 2018
Time: 4:30-5:30 pm
Location: 208 Clark Hall

Students, meet the speaker over coffee and cookies in the Bennett Conference room at 3:30 pm