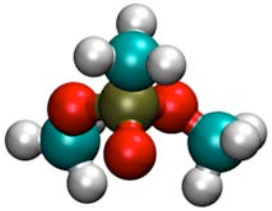
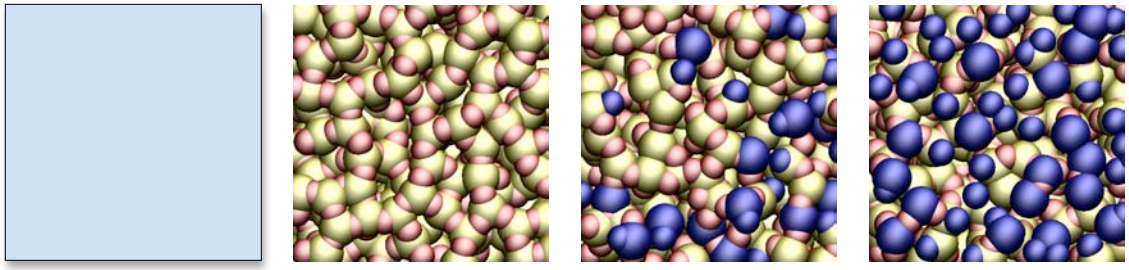
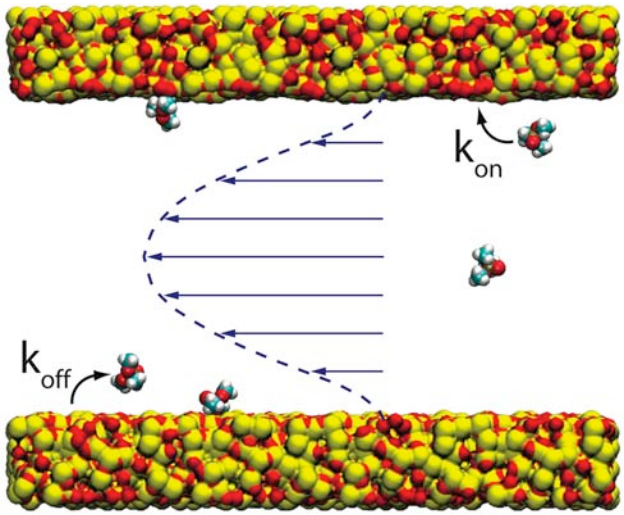
Multiscale Model of a Flow through a Silica Nanogap



a small organic molecule dimethylmethyl-phosphonate (DMMP) is used for method development

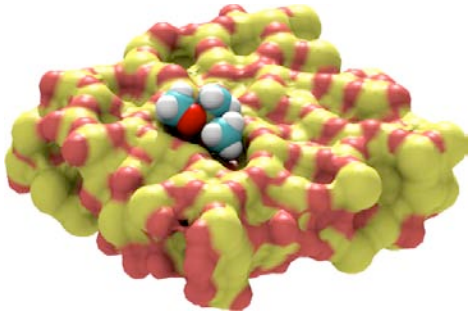


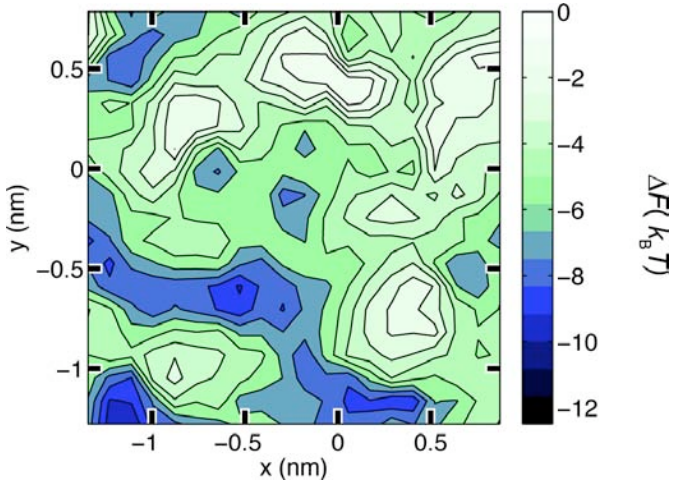
Model is tested using silica surfaces of different roughness and hydrophobicity



Atomistic simulation of solute's flow through silica nanogap

We developed a general method for simulation of sorption/desorption phenomena at a liquid-solid interface. Using realistic, atom-resolution simulations, we examined sorption/desorption of a prototypical solute from silica surfaces of different properties. The atomic-scale simulation were related to the macroscopic behavior by computing a 3-D map of the solute's interaction with the surface and the flow profile. Our method will find applications in modeling nanofluidic devices and oil extraction procedures.





3D potential of mean force describes interaction of DMMP with the nanogap