

Abstract Submitted  
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**Effect of surface wettability on liquid structure and mobility near a solid surface** J.A. THOMAS, A.J.H. MCGAUGHEY, Carnegie Mellon University — Using molecular dynamics and Langevin dynamics simulations, we study how surface wettability affects the density, structure, diffusion, and migration of a monatomic liquid near a solid surface. The liquid atoms near the solid surface experience different dynamics than those in the bulk. The resulting structure and density variations generate an anisotropic self-diffusion coefficient tensor which, in theory, can be tuned to bias liquid movement towards or away from the surface. The self-diffusion coefficient parallel to the surface is found to be inversely proportional to the local liquid structure factor and the self-diffusion coefficient parallel to the solid surface is found to be proportional to the local liquid density. These findings suggest that altering the wettability of a micro/nanochannel could provide a means for passive control of the diffusion of select targets towards a functionalized surface.

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