Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

A water flow molecular dynamics simulation in a methyl functionalized imogolite nanotube NATHAN CANNON, TAKUMI HAWA, The University of Oklahoma — Some nanotubes have enhanced water transport properties, but the imogolite nanotube, which is a hydrous aluminosilicate nanotube, is not known to and we suspect that it does not. To achieve enhanced water transport, its inner surface was made hydrophobic by replacing an OH group with a CH3 group. The performance of the natural and modified imogolites was measured by inducing water flow and comparing the results with continuum theory using molecular dynamics simulations to determine transport efficiency. Simulations were run using the CLAYFF and CVFF potentials for the nanotube and the SPC/e model for water. The natural imogolite performed 200 times worse than continuum theory, while the modified imogolite performed 10 times better. We also investigated the interaction of the inner surface atoms with the water molecules to help to explain what factors are the most influential in effecting the transport of water.

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Date submitted: 14 Nov 2013 Electronic form version 1.4