Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Dynamics of H_2O Molecules Confined in Fullerenes ROXANNE TUTCHTON, PAUL LARSON, ZHIGANG WU, The Colorado School of Mines —
Structural and dynamical properties of confined water in nanostructures are expected to be remarkably different than those of bulk water. Water confined in nanotubes and graphene sheets has been extensively investigated theoretically, yet very few computational efforts have been made to study confined water in fullerenes though, experimentally, water molecules have been successfully encapsulated inside fullerenes as small as C_{60}. In this work, we carry out classical molecular dynamics simulations to investigate density and H-bond distributions inside fullerenes ranging from C_{60} to C_{540}. Our results show that as the size of the fullerene increases, concentric shells of water molecules are formed, and the water density is higher than that of bulk water while the average H-bond per molecule is slightly lower than the bulk value. We also find that these shells of H_2O are solid-like at room temperature, but they should eventually become liquid-like at high temperatures.

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Date submitted: 15 Nov 2013 Electronic form version 1.4