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Fast Rotation of a Single Water Molecule in Buckyball AMIR BARATI FARIMANI, YANBIN WU, NARAYANA ALURU, Mechanical Science and Engineering, Beckman Institute, University of Illinois at Urbana-Champaign — Successful encapsulation of a single water molecule in C60 by Kurotobi and Murata (Science, 333, 2011) opens up an opportunity to study non-hydrogen bonded single water molecule. Here, we investigate the properties of a single water molecule in buckyball by using molecular dynamics (MD) and density functional theory (DFT). By using DFT, we found that there's a shift of 23 cm^{-1} in vibrational frequencies of O-H bond of water molecule when it's inside C60. By using MD, we compute the rotational diffusion and entropy of water. Our findings show that water rotates about an order of magnitude faster compared to a single water molecule in bulk. While $\text{H}_2\text{O}@\text{C60}$ has near zero translational entropy, its rotational entropy is 6.5 times larger than rotational entropy of bulk water.

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