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Slow Relaxations of Supercooled Water Determined by Energy Landscape Sampling NATHAN WALTER, YANG ZHANG, Univ of Illinois - Urbana — Molecular Dynamics simulations have been widely used to provide insight into atomistic scale materials behavior and to compare with neutron scattering experiments. However, such simulations are inhibited by temporal scale and spatial scale constraints. As a consequence, it is only possible to predict the dynamical behavior of materials at short times, while atomistic simulations beyond microsecond remain a challenge. The energy landscape sampling methods have been suggested to predict materials behavior at long times. Herein, we show that by efficiently sampling the activation barriers of the high-dimensional energy hypersurface we were able to study the slow dynamics of supercooled ST2 water down to deeply supercooled temperatures. Furthermore, the method allows us to quantify the statistics of the activation barriers, yielding insight into the slow and fast dynamics of ST2 water at low temperatures. The computed transport coefficients across a wide temporal range are useful to bridge the gap between neutron scattering experiments and other bulk measurements.

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