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Two-State Dynamics in Liquids and Glass on a Picosecond Timescale MARCUS CICERONE, MIAOCHAN ZHI, NIST, JUAN DEPABLO, University of Chicago — We present results from neutron scattering, atomistic MD simulations, and optical Kerr effect spectroscopy (OKE) to demonstrate that liquids and glasses exhibit two dynamic states at short times. We provide evidence that the two dynamic states arise from molecules that are either tightly caged or loosely caged on a ps timescale. This heterogeneous motion is associated with hopping at low temperature, but the two-state scenario persists well above the melting point, and also contributes significantly to transport at the higher temperatures. Using concepts derived from this model we are able to quantitatively predict self-diffusion of small molecule glassformers well into the supercooled regime.

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