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Theoretical Insights from Facile Microsecond Simulation of the Glass Transition[1] JUI-HSIANG HUNG, TARAK PATRA, DAVID SIMMONS, Univ of Akron — Despite more than half a century of research, the fundamental nature of the glass transition remains one of the major open questions in polymer science and condensed matter physics. Molecular dynamics simulations have provided key insights into this problem, but their ability to firmly establish the underlying nature of glass formation have been limited by the extreme computational difficulty of directly probing the deeply supercooled regime most relevant to this process. Here we describe a new protocol for simulation of the glass transition enabling facile access to in-equilibrium segmental relaxation times approaching and exceeding one microsecond – well into the deeply supercooled regime of most glass-forming liquids. Coupled with a well-validated strategy for extrapolation to experimental timescales, this approach provides vastly improved prediction of experimental glass transition temperatures. Here we combine data acquired through this protocol for the deeply supercooled regime of polymeric, inorganic, organic, and metallic glass formers to robustly test several theories of glass formation and identify microscopic phenomenological features shared across all classes of glass-forming liquid in the deeply supercooled regime.

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