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Quantitative relaxation dynamics of supercooled liquids from first principles LIESBETH JANSSEN, Columbia University, PETER MAYER, ThinkEco, Inc., DAVID REICHMAN, Columbia University — Understanding the liquid-to-glass transition remains one of the deepest unsolved problems in condensed matter science. Here we present a novel first-principles framework, referred to as generalized mode-coupling theory (GMCT), which can predict the microscopic dynamics of glass-forming systems with near-quantitative accuracy using only simple static information as input. The theory is based on the well-established standard mode-coupling theory (MCT) of the glass transition, but rigorously incorporates higher-order dynamic density correlations neglected in standard MCT. We demonstrate that GMCT can accurately describe the dynamics of quasi-hard spheres over an unprecedentedly large time and density domain, supporting the view that activated glassy behavior is inherently dynamic in origin. Finally, our schematic results show that GMCT is capable of predicting novel types of glass transitions, including type-A, type-B, and avoided transitions, as well as different types of relaxation-time scaling behaviors. This suggests that GMCT may constitute the first microscopic, first-principles theory that can account for different fragilities in glass-forming materials.

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