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Progress Towards Atomistic Simulations that Reach Anthropological Timescale and Beyond

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Atomistic and first-principles modeling, which describe the world as assembly of atoms and electrons, provide the most fundamental answer to problems of materials. However, they also suffer the most severe timescale limitations. For instance, in molecular dynamics (MD) simulations, in order to resolve atomic vibrations, the integration time step is limited to hundredth of a picosecond, and therefore the simulation duration is limited to sub-microsecond due to computational cost. Although a nanosecond simulation is often enough (surprisingly) for many physical and chemical properties, it is usually insufficient for predicting microstructural evolution and thermo-mechanical properties of materials. In this invited talk I will discuss recent attempts at overcoming the timescale challenges of atomic-resolution simulations: (a) strain-boost hyperdynamics [Phys. Rev. B 82 (2010) 184114] for simulating primarily displacive events and associated issues of activation entropy and the Meyer-Neldel compensation rule, (b) diffusive molecular dynamics (DMD) [Phys. Rev. B 84 (2011) 054103] for microstructural evolution driven by repetitive diffusion events and coupled displacive-diffusive processes, and (c) a Markovian network statistical mechanical treatment of the energy-landscape basin connectivity and a formula for the viscosity of supercooled liquid and glass [PLoS ONE 6 (2011) e17909]. Challenges and future directions are discussed.