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Atomistic Modeling and Simulation of Long-Term Transport Phenomena in Nanomaterials

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In the past two decades, extensive research has been conducted towards developing nanomaterials with superior transport properties, such as heat conductivity and mass diffusivity, for applications in various industries including, but not limited to, energy storage and microelectronics. In terms of modeling and simulation, a long-standing difficulty lies in the separation of temporal and spatial scales. Indeed, many transport phenomena in nanomaterials are characterized by slow kinetic processes with time scale of the order of seconds, hours, or even years, far beyond the time windows of existing simulation technologies such as molecular dynamics (MD) and Monte Carlo (MC) methods. To resolve this issue, we propose a novel deformation-diffusion coupled computational framework that allows long-term simulation of such slow processes, while at the same time maintains a strictly atomistic description of the material. Specifically, we first propose a theory of non-equilibrium statistical thermodynamics for multi-species particulate solids based on Jayne's maximum entropy principle and the meanfield approximation approach. Unlike in MD and MC, here thermal oscillations and the individual hops of atoms are not tracked explicitly, but instead accounted for in a statistical sense. This non-equilibrium statistical thermodynamics model is then coupled with discrete kinetic laws, which govern mass diffusion and heat conduction at atomic scale. In this talk, we explore the capabilities and performance of this computational framework through its application to two active research topics in nanotechnology: hydrogen storage in metal nanofilms, and heat conduction in Si nanowires.

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