Simulating transport properties of superionic materials

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In this talk I will discuss recent advancements in the atomistic theory and simulation of transport properties (ionic diffusivity, heat and charge transport) of superionic materials, i.e., systems characterized by one or more species diffusing through a solid matrix. By leveraging the Green-Kubo theory of linear response [1], I will show how to combine fundamental invariance principles of transport coefficients with advanced topics on the quantum theory of matter to obtain ab-initio accurate thermal [2] and electrical [3] conductivities for these materials. I will also compare different statistical techniques based on the analysis of time series that can be used in practice to extract transport coefficients from equilibrium molecular dynamics simulations [4]. Examples will be given for paradigmatic materials for energy (e.g., solid-state electrolytes) [5] and planetary science (e.g., superionic water at Uranus' interior conditions) [6]. Finite-size effects due to the limited size of the simulation box will be extensively covered and showcased for several materials representative of type I and type II superionic conductors [7].

References:

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