From ab-initio to model systems: tales of unusual conductivity in electronic systems at high temperatures

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In this talk, two systems with unusual conductivity at high temperatures will be discussed. First, we highlight our numerical prediction of a new superionic phase in high-temperature, high-pressure ice. This phase is an electronic insulator, but an ionic conductor with highly anisotropic diffusion. Second, we describe a model system with zero conductivity even at infinite temperature, a phenomenon commonly known as many-body localization (MBL). We demonstrate a new method for efficiently and compactly representing the complete spectra of MBL states and show how the phenomenology of MBL follows directly from the properties of these excited states.