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Computational screening and design of new materials for energy storage and conversion: batteries and thermoelectrics BORIS KOZINSKY, Bosch Research, Cambridge MA — Understanding the atomic-level origins of thermoelectricity is necessary for the design of higher-performing materials, and we demonstrate that ab-initio computation is a valuable tool. By developing and using advanced methods to compute intrinsic contribution to electron lifetimes from electron-phonon coupling, we are able to predict temperature and doping dependence of electronic transport properties in doped semiconductors. We combine these tools to perform rapid screening of new thermoelectric compositions. In energy storage, a promising path to enabling safe high-energy-density batteries is the introduction of inorganic solid electrolytes that can protect the Li-metal anode. We have achieved a detailed understanding of a promising class of garnet compounds by developing a set of efficient atomistic computational techniques to analyze structure ordering and ionic transport mechanisms. These methods allow us to map the transport phase diagram of a broad range of compositions and to predict new phases and phase transitions. The computational techniques are coupled with a novel software platform AiiDA that combines high-throughput automation with data analysis capabilities.

Boris Kozinsky
Bosch Research, Cambridge MA

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