

# **New energy materials from data-driven computations of transport properties**

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This talk will illustrate how technologically relevant materials for energy storage and conversion can be designed and discovered starting with fundamental physical understanding, development of transferrable electronic structure and atomistic algorithms and deployment of new automation and informatics tools to rapidly investigate a wide range of candidate compounds. A particularly important challenge and an opportunity is the development of accurate computational methods and descriptors for transport properties, given their high sensitivity to materials' structure and composition. One example is the thermoelectric energy conversion, where materials operate due to the quantum-level coupling of electronic and thermal carriers. In the domain of ionic transport, computations can provide crucial insight for the design of solid-state electrolytes for next-generation electrochemical systems.