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High throughput ab-intio modeling of proton transport in solid electrolytes JANAKIRAMAN BALACHANDRAN, LIANSHAN LIN, PANCHAPAKESAN GANESH, Oak Ridge National Labaratory — Solid oxide materials that can selectively transport protons have great potential for fuel cell applications. However several fundamental questions remain unanswered such as (a) How do the dopants organize at various dopant concentrations, (b) How spatial organization of dopants influence proton migration energy, (c) How disorder and strain in a material influence its ionic transport. \In this work have developed an integrated high throughput framework to calculate proton transport properties by integrating open source packages (such as pymatgen, fireworks) The high throughput framework scales well on supercomputing clusters. We have used this framework to analyze over 100 perovskites compounds with over 12 different dopant atoms. These computational models enable us to obtain insights how the proton transport properties depend on host and dopant atoms. Further, we also perform ab-initio modeling to understand how dopants spatially organize at different dopant concentrations, and how this spatial organization affects proton conductivity. This analysis enabled us to obtain fundamental insights on why proton conductivity decreases in Y doped BaZrO3 at high dopant concentrations.

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