Holistic computational structure screening of more than 12,000 candidates for solid lithium-ion conductor materials[1] AUSTIN D. SENDEK, QIAN YANG, EKIN D. CUBUK, KAREL-ALEXANDER N. DUERLOO, YI CUI, EVAN J. REED, Stanford Univ — We present a new type of large-scale computational screening approach for identifying promising candidate materials for solid state electrolytes for lithium ion batteries that is capable of screening all known lithium containing solids. To predict the likelihood of a candidate material exhibiting high lithium ion conductivity, we leverage machine learning techniques to train an ionic conductivity classification model using logistic regression based on experimental measurements reported in the literature. This model, which is built on easily calculable atomistic descriptors, provides new insight into the structure-property relationship for superionic behavior in solids and is approximately one million times faster to evaluate than DFT-based approaches to calculating diffusion coefficients or migration barriers. We couple this model with several other technologically motivated heuristics to reduce the list of candidate materials from the more than 12,000 known lithium containing solids to 21 structures that show promise as electrolytes, few of which have been examined experimentally. Our screening utilizes structures and electronic information contained in the Materials Project database.

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