Predicting Na-ion diffusivity in glass electrolytes with compact, interpretable descriptors

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Glass electrolytes are promising candidates for solid-state sodium batteries, but understanding how their composition and atomic structure govern ionic transport remains challenging. Here, we combine machine-learning prediction with feature selection to establish a compact, physically interpretable description of temperature-dependent Na-ion diffusivity. Using a published dataset of 1302 glass compositions with simulated diffusivities at multiple temperatures [1], we compare atomistic representations based on the smooth overlap of atomic positions (SOAP) [2] with physicochemically motivated descriptors capturing composition, packing, local coordination, and migration-network geometry. Kernel ridge regression (KRR) and neural-network (NN) models were used to predict Na diffusivity from these representations and temperature, without imposing an Arrhenius functional form. Building on this result, we use mutual information (MI) [3] to assess their relevance and redundancy, identifying a reduced descriptor set that preserves predictive accuracy on independent glass compositions without substantial loss. These findings demonstrate that a compact representation can capture much of the information relevant to Na-ion diffusion, supporting efficient screening of glass electrolytes and providing insight into their structure–transport relationships.

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References

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