ABSTRACT:

Accelerating Materials Discovery: The Role of Interpretable Machine Learning in Unveiling New Proton-Conductive Electrolytes

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The discovery and exploration of new materials, crucial for advancing science and technological innovation, traditionally rely on researchers' intuition. However, the success rate remains low due to the need to identify function-specific materials from vast candidate pools. Even when utilizing recent high-throughput calculations and machine learning techniques, issues with low prediction accuracy persist. Here, we use interpretable machine learning models to accelerate the discovery of new proton-conductive electrolytes. The first discovery, SrSn0.8Sc0.2O3Hx, was made in a single trial, using hydration reaction data. Incorporating physicochemical rules of hydration into descriptors, we accurately predicted the temperature-proton concentration relationship in a wide range of perovskite oxides. The second discovery, the first proton-conductive electrolyte composed solely of p-block cations in Pb-doped Bi12SiO20Hx, also occurred in a single trial, using high-throughput first-principles calculation data and machine learning models. Notably, this crystal structure represents a first in the field of proton conductors. Both cases underline the critical role of integrating point defects into machine learning models, a key to boosting the success rate in the quest for new materials.

[1] S. Fujii, Y. Shimizu, J. Hyodo, A. Kuwabara*, Y. Yamazaki*, Discovery of unconventional proton-conducting inorganic solids via defect chemistry-trained, interpretable machine learning, preprint on ChemRxiv.
[2] J. Hyodo, K. Tsujikawa, M. Shiga, Y. Okuyama, Y. Yamazaki*, Accelerated discovery of proton-conducting perovskite oxide by capturing physicochemical fundamentals of hydration, ACS Energy Letters, 6(2021), 2985-2992.