A Machine Learning Approach to Cation Identification for Solubility Optimization of Redox Active Material for Non-aqueous Redox Flow Batteries

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Renewable energy integration into power grids necessitates efficient energy storage solutions, with non-aqueous redox flow batteries (NRFBs) emerging as promising candidates due to their wider temperature range and higher energy density than aqueous counterparts. However, the optimization of NRFBs is hindered by the challenge of identifying soluble cations, a crucial factor in maximizing energy density. In this study, we demonstrate the transformative potential of machine learning in expediting the discovery of soluble cations for NRFBs. Specifically, through the training of regression models, we predicted the solubility of 500 quaternary ammonium cations. Our findings reveal the superior performance of ensemble methods in accurately predicting cation solubility compared to traditional regression models. This streamlined approach to NRFB material discovery holds significant implications for advancing sustainable energy solutions, offering a cost-effective pathway towards the widespread adoption of renewable energy sources in power grids.