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Machine Learning-Accelerated Discovery of Sustainable Redox-Active Polymers for Next-Generation Batteries

Owing to urgency in reducing the global carbon footprint and ease climate change, global governments reached a decisive accord to promote sustainable practices. This entails replacing fossil fuels with devices like electric batteries. At present, electric batteries rely on transition metals as a crucial component. However, the production of these transition metals involves intense mining operations, which in turn emanates significant pollutants. Endeavoring to clamp down on this, there is a need for polymeric materials to be used as electrode materials in batteries, owing to their lower carbon footprint. In our research, we use Machine Learning techniques to identify and optimize polymeric materials for batteries. The ML model's efficiency in identifying suitable polymeric materials will surpass random searches and base models in terms of accuracy and speed. In our research, we collect data pertaining to batteries based on redox active polymers, and train the ML model on battery properties like voltage, specific capacity etc. Post training, the model is screened on a library of candidates to identify suitable redox-active polymers for batteries. The most suitable polymeric materials that are screened will be passed on to experimentalists to validate and match the properties that we predict. In an attempt to improve predictions, several other approaches will be taken like employing transfer learning from molecules to polymers or including DFT derived (proxy) properties in the data.