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Artificial intelligence and machine learning in energy storage and conversion

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Artificial intelligence (AI) and machine learning (ML) have been transforming the way we perform scientific research in recent years.[1–4] This themed collection aims to showcase the implementation of AI and ML in energy storage and conversion research, including that on batteries, supercapacitors, electrocatalysis, and photocatalysis. The works covered range from materials, to devices, to systems, with an emphasis on how AI and ML have accelerated research and development in these fields.

Currently, most design principles in energy chemistry are empirical in nature due to the complexity of material and device synthesis. To solve this challenge, ML models can be trained using experimental and computational data to construct more quantitative structure–property relationships. In a review, Xu *et al.* (**https://doi.org/10.1039/D3YA00057E**) discuss the application of ML in diverse areas like batteries and catalysis, and how ML can aid the fabrication of new materials and devices.

There are many promising battery materials waiting to be discovered, but the large chemical space makes trial-and-error methods intractable. Ng *et al.* (**https://doi.org/10.1039/D3YA00040K**) provide an overview of the use of ML to predict material properties and discover new electrode/electrolyte materials. The three main strategies of ML are covered, namely direct property predictions, machine learning potentials, and inverse design, for the future development of sustainable batteries.

Organic batteries are known to be eco-friendly and cost-effective, but performance predictors of such batteries are lacking in the field. In a work by Tobita *et al.* (**https://doi.org/10.1039/D3YA00161J**), a new capacity predictor was devised for organic anode-active materials using sparse modeling and domain knowledge. The new model was not only generalizable and interpretable, but also superior in terms of the high prediction accuracy and small amount of training data used.

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Amorphous porous carbons are common electrode materials for supercapacitors due to their high conductivity and low cost. ML methods have been used to predict capacitance, but the lack of physical inputs may result in incorrect predictions at high charge–discharge rates. Pan *et al.* (**https://doi.org/10.1039/D3YA00071K**) reported a physics-based Gaussian process regression technique to predict the capacitance of carbon electrodes, which was found to work better than conventional ML methods.

Moving on to catalysis, the carbon dioxide reduction reaction is a potential approach to combat climate change and produce chemicals sustainably, but the reaction mechanisms behind C_2 product formation remain poorly understood. Gariepy *et al.* (**https://doi.org/10.1039/D2YA00316C**) integrated density functional theory and ML to investigate the adsorption of a key *COCOH intermediate on eight different Cu-based binary alloy catalysts to find the optimal candidates with the weakest adsorption energy.

Oxidative coupling of methane is another promising method to synthesize C_2 hydrocarbons, and high-throughput experimentation has been traditionally used to discover new catalyst materials. In an *in silico* work, von Meyenn *et al.* (**https://doi.org/10.1039/D2YA00312K**) combined directed evolution and ML to design new catalysts for oxidative methane coupling using a genetic algorithm. The C_2 yield of the catalysts was then evaluated using a random forest algorithm to propose promising candidates.

We hope that these works have given you an idea of the state-of-the-art progress and will inspire you to pursue the opportunities in this burgeoning field of ML and sustainability.

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