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## Flow Battery DFT

Are aqueous organic redox flow batteries suitable for low energy density?

Aqueous organic redox flow batteries (AORFBs) face challenges of low energy density, which can be addressed by the strategy of redox-targeting (RT) reaction integrating solid materials (SMs) with redox mediators (RMs). However, the potential matching between SM and RM is demanding and complex.

Are redox flow batteries good for energy storage?

Among various energy storage systems, redox flow batteries (RFBs) are promising techniques for large-scale energy storage due to attractive characteristics of decoupled energy and power, high scalability, design flexibility and long cycling ,,,

Do all-liquid redox flow batteries need a higher energy density?

A main issue for all-liquid RFBs however is their low energy densities ( $\sim 50 \text{ Wh L}^{-1}$  for the vanadium redox flow battery). For scaling up the energy, an electrolyte couple with higher energy density (higher concentration or cell potential) or a larger quantity of electrolyte is needed.

Are transition metal complexes suitable for redox flow batteries?

For complexes with similar ligands, potentials calculated using simple implicit solvation models could be corrected using linear regression (MAE=0.051 V). Transition metal complexes are a promising class of redox mediators for targeting redox flow batteries due to the tunability of their electrochemical potentials.

A robust anionic sulfonated ferrocene derivative for pH-neutral aqueous flow battery. Energy Storage Materials 2020, 29, 216-222. 14. Ji, Y.; Zhang, F.; ...

Solvent treatment has been proved to be an effective strategy for the preparation of highly selective porous membranes for flow batteries. Herein, a fast and efficient method to ...

The aqueous organic redox flow batteries (AORFBs) were first proposed by Huskinson and Aziz of Harvard University in 2014 [1]. In the past six years, they have been ...

Effective utilization of thermal energy is attracting attention for the realization of a carbon-neutral society. To convert thermal energy into electrical energy, we recently proposed ...

These methodologies, proven effective in expediting material designs and optimizations across various fields, excel in exploring and ...

DFT) calculations were performed to further reveal the interaction between porous membrane and various solvents. The structure of PBI segment, PBI-10 and solvents were ...

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