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This study utilized density functional theory (DFT) with the B3LYP functional and 6-31G (d) basis set to calculate the first and second reduction potentials of benzoquinones (BQ).

In this study, DFT calculations are applied to determine the main factors for designing organometallic redox flow battery chemicals. Several metals and ligands were ...

LCC researcher, Assistant Professor Ya Ji "s Group recently published a paper on "Potential prediction in aqueous organic redox-targeting flow batteries: DFT calculation and ...

A data-driven and DFT assisted theoretic guide for membrane design in flow batteries

A flow battery, or redox flow battery (after reduction-oxidation), is a type of electrochemical cell where chemical energy is provided by two chemical components dissolved in liquids that are ...

Organic redox flow batteries are promising for grid stabilisation, but the insufficient ion separation by membrane separator can limit the lifetime and increase the cost.

In this study, we focused on the redox potential of ferrocyanide/ferricyanide in six different solvents (water, ethanol, acetone, ...

In the context of the search for new organic electrolytes for redox flow batteries, we present and validate a robust procedure to calculate the redox potentials of organic molecules at any pH ...

In this study, we focused on the redox potential of ferrocyanide/ferricyanide in six different solvents (water, ethanol, acetone, 1-butanol, acetonitrile, and dimethyl sulfoxide ...

In this study, DFT calculations are applied to determine the main factors for designing organometallic redox flow battery chemicals. ...

Herein, a computational predictive tool for redox flow batteries based on NBO and ADCH charge distribution studies is presented and supported by experimental evidence.

Organic redox flow batteries are promising for grid stabilisation, but the insufficient ion separation by membrane separator ...

To further accelerate the design of new improved batteries, a computational approach was used in order to assess their structural stability. The results show that the proposed compounds are ...

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