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3D KINETIC MONTE CARLO MODELING OF THE ELECTROCHEMICAL INTERFACE IN RFB

This three-dimensional model based on kinetic Monte Carlo, is developed to study the electrode-anolyte interface of a methyl viologen-based organic redox flow battery. This model captures various electrode processes, such as ionic displacement, electron transfer and degradation of active materials.

The workflow consists of input parameters obtained from density functional theory calculations, and a kinetic Monte Carlo algorithm to simulate the discharging process and electric double layer model to account for the electric field distribution near the electrode surface. Galvanostatic discharge was simulated at different anolyte concentrations and input current densities, which demonstrated that the model captured the formation of the electrical double layer due to ionic transport. The simulated electrochemical kinetics (potential, charge density) were found to be in agreement with the Nernst equation and the obtained EDL structure corresponded with published molecular dynamics results. The model's flexibility allows further applications of simulating the behavior of different redox couples and makes it possible to consider other molecular-scale phenomena.

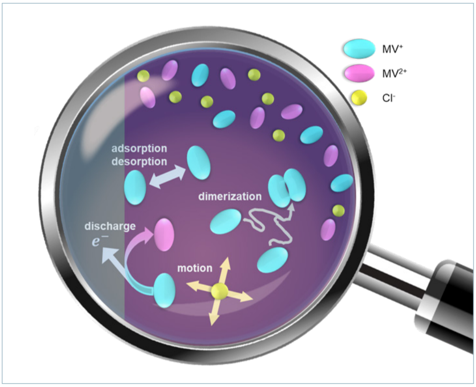
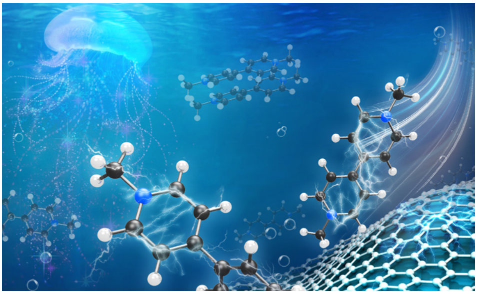


Illustration of the targeted simulation system and various events happen on the electrode-electrolyte interface.



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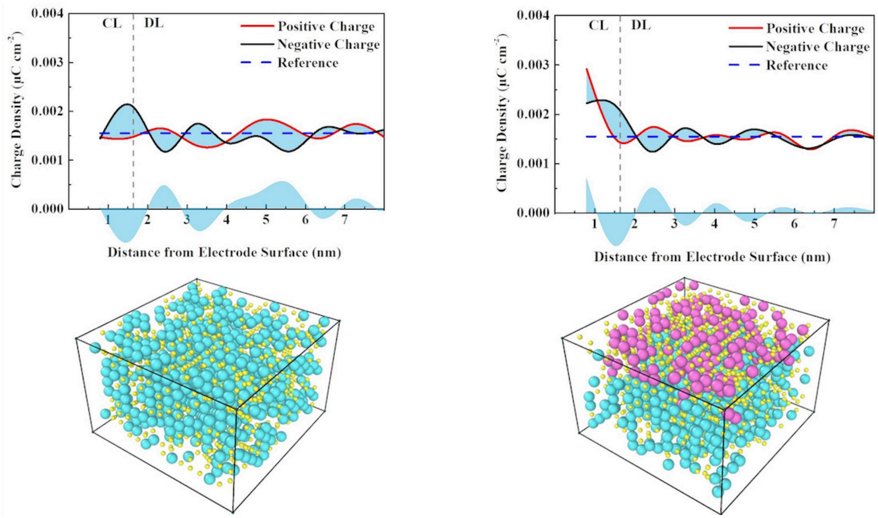

The model was used to simulate galvanostatic discharge at different anolyte concentrations and input current densities. The EDL formation was captured through the simulations, which demonstrated a substantial impact on ionic transport and electrode kinetics. Furthermore, the obtained EDL structure of charge inversion was found to correspond to the results reported in literature for other systems based on the Molecular Dynamics approach.

The model demonstrates that the interplay between the electrostatic impact and the electrochemical kinetics determine the final steady-state of the system, and the charge density at the electrode influences the system configuration, which determines the discharge rate and the electrode potential. The model’s flexibility allows further applications of simulating the behavior of a target redox flow couple in an ORFB. With the help of DFT calculations, electrochemical kinetics can be obtained with simple experiments. The structure of this model also makes it possible to consider other events when needed.

[Ref] J. YU et al, Small, 07.2022

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