PÔSTER - RESUMO - DISPOSITIVOS ELETRÔNICOS, ELETROQUÍMICOS, SUPERCAPACITORES E BATERIAS

ON THE PERFORMANCE OF MXENE-ELECTROCHEMICAL SUPERCAPACITORS CONTAINING DEEP EUTECTIC SOLVENT AS ELECTROLYTES

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The global surge in demand for efficient and sustainable energy storage solutions has catalyzed significant interest in supercapacitors, especially for applications requiring fast charge–discharge rates. MXenes, an outstanding class of two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, have emerged as exceptional electrode materials that enable enhanced ion accessibility and capacitance through a mixture of electric double-layer and pseudocapacitive mechanisms.[1] Concomitantly, deep eutectic solvents (DESs) have gained prominence as sustainable alternatives to conventional electrolytes. Formed via hydrogen-bond donor–acceptor pairs, DESs offer favorable features: biodegradability, low volatility, straightforward synthesis, and broad electrochemical stability windows, offering a cost-effective and environmentally friendly option for energy storage applications.[2] Despite progress in both materials, the interfacial structure and dynamics between MXenes and DESs remain underexplored. The intricate behavior governed by hydrogen-bond networks in DESs, combined with the complex surface terminations of MXenes, warrants a detailed atomistic understanding to optimize charge storage and overall device performance.[1] Molecular dynamics

(MD) simulations, particularly those employing constant-potential methods, are powerful tools to probe such interfacial structures and processes with atomic precision. In this work, we conduct comprehensive constant-potential MD simulations to analyze the behavior of DESs confined between MXene electrodes. Our approach includes: (i) structural examination of interfacial layering and hydrogen-bond networks, (ii) dynamical analysis of solvent orientation and ion mobility, and (iii) evaluation of charge accumulation and differential capacitance modulation by surface functional groups. From our study, we figure out how DES interacts with MXene surface terminations and the interplay to electrochemical performance. Aspiring to bridge theoretical predictions with practical applications, our findings contribute foundational insights and design guidelines for the development of high-performance, sustainable supercapacitors leveraging MXene–DES architectures.

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[1] Recent Advances in MXenes for Supercapacitors. Journal of Materiomics 2023, 9, 1234–1250.

[2] Deep Eutectic Solvents: Properties and Applications in Electrochemistry. Current Opinion in Green and Sustainable Chemistry 2023, 39, 100745.

Palavras-chave: deep eutectic solvents; mxenes; supercapacitors; energy storage.