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Locally Concentrated Electrolytes for Al-S Batteries, a Molecular Simulation Investigation

Locally Concentrated Electrolytes for Al-S Batteries, a Molecular Simulation Investigation

Aluminum-sulfur (Al-S) batteries are emerging as a promising alternative to lithium-ion (Li-ion) batteries due to their lower cost, safety, and environmental advantages[1-2]. Aluminum, being abundant and less reactive than lithium, enhances battery stability and affordability, making Al-S batteries suitable for energy storage[3]. However, challenges like electrolyte viscosity and aluminum reactivity must be addressed. Room- temperature ionic liquids and deep eutectic solvents (DES) based on AlCl3 show potential for improving electrolyte performance. Adjusting the AlCl3 ratio in these electrolytes influences ionic composition[4], crucial for efficient aluminum plating and stripping. The addition of low-viscosity cosolvents like 1,2- difluorobenzene (dFBn) helps mitigate viscosity issues, enhancing battery efficiency.

[1] Nature 2015 520 325-328, [2] Chemistry Select 8 (10) 2023 me202204575 [3] J. Phys. Chem. C 2017, 121 (48), 26607−26614 [4] ECS Transactions, 2020, 98 (10), 129-139. Our purpose here is to present, as far as we know for the first time, the results obtained from a set of simulations of the two electrolytes Emim:AlCl3:dFBn and Urea:AlCl3:dFBn. In particular, we have studied the structure and the dynamics of the two liquid electrolytes using molecular dynamics (MD) and investigating the dependence of their properties both on the composition and on temperature

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