

# Hydrogen Bonding in Water-Modified Solvate Ionic Liquids Studied by Molecular Dynamics Simulations

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Lithium-based batteries rank among the most promising energy storage technologies due to their high energy densities. However, conventional electrolytes often suffer from high flammability and limited electrochemical stability. Solvate ionic liquids (SILs), formed by mixing lithium salts of weakly coordinating anions (e.g., [Li][NTf<sub>2</sub>]) and molecular solvents like triglyme, have emerged as safer alternatives. For certain compositions, lithium forms stable 1:1 complexes with triglyme, reducing ion pairing and enhancing ionic transport [1].

To further improve transport properties, we explore the addition of water to this SIL system via molecular dynamics simulations. This approach combines features of SILs and water-in-salt (WIS) electrolytes. We find that water can partially or fully replace triglyme in the lithium coordination shell depending on composition. Water also forms hydrogen bonds with displaced triglyme and [NTf<sub>2</sub>]<sup>−</sup> anions, spatially isolating water molecules and disrupting bulk-like water behavior. This hydrogen-bond-mediated shielding enhances ion mobility while preserving the electrochemical benefits of SILs. However, exceeding a critical water content results in water–water hydrogen bonding and cluster formation, reintroducing bulk water characteristics and narrowing the electrochemical window.

Our study demonstrates that hydrogen bonding plays a key role in controlling the structure and transport properties of hybrid electrolytes. By carefully balancing lithium coordination and hydrogen bond interactions, it is possible to design electrolytes that unify the strengths of SILs and WIS systems while mitigating their limitations.

## References

[1] J. K. Philipp, L. Kruse, D. Paschek, R. Ludwig, J. Phys. Chem. B, 2025, 129, 22, 5561–5577.

## Keywords

Hydrogen bond: medium; State of system: liquid/solution

## This abstract is submitted for....

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