

## Special Issue

# Computational Studies of Ionic Liquids and Their Analogues

### Message from the Guest Editors

Dear colleagues, This Special Issue will explore the latest advances in the computational modelling of ILs and DESs, aiming to deepen our understanding of their complex behaviour. The methods include, but are not limited to, classic and ab initio molecular dynamics simulations, density functional theory, Monte Carlo methods, Cosmo-RS, and machine learning approaches. Through this collection, we aim to showcase the potential of computational chemistry to revolutionize the development and application of these next-generation solvents. Dr. Iuliia V. Voroshylova

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### Guest Editors

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### Deadline for manuscript submissions

closed (30 September 2025)



## International Journal of Molecular Sciences

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