EXPERIMENT AND QUANTUM CHEMICAL CALCULATION FOR THE REMOVAL OF WATER POLLUTANTS USING IONIC LIQUID AND DEEP EUTECTIC SOLVENT





(Emerging Pollutants and Managing Wastewater and Waste)

COSMO-RS Model



To evaluate the molecular behavior of water pollutants using Ionic Liquids (ILs) and Deep Eutectic Solvents (DESs) using σ – Profile and σ – Potential

Solution Thermodynamics Properties

To study the pure compound and their binary mixture [ILs/DESs (1) + water pollutants (2)] behavior at different concentration and different temperatures from 293.15 K – 343.15 K.

Solvent Extraction Process

To determine the quality of water matrices in terms of distribution coefficient (D) and extraction efficiency ($\%\eta$)

Feasibility Studies

To study the thermodynamic feasibility of green solvent-based extraction process at different temperatures in terms of change in Gibbs free energy, change in enthalpy, change in entropy





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