# Modeling and Simulation of Deep Eutectic Solvents for Energy Applications

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The design of sustainable materials for energy applications represents a significant challenge in the quest for a circular economy. This study introduces an innovative method for waste lithium-ion batteries (LIBs) utilizing an eco-friendly deep eutectic solvent (DES) composed of glycine, ascorbic acid, and water. A comprehensive approach was adopted, incorporating advanced factorial design, kinetic modeling, and machine learning to fine-tune process parameters and maximize leaching performance. The extraction kinetics were found to be driven mainly by endothermic surface reactions, with activation energies measured at 81.5 kJ/mol for cobalt and 110.9 kJ/mol for lithium. An ensemble neural network model accurately predicted the extraction process, achieving an $R^2$ value greater than 0.95. This indicates the strength of the computational methodology. Density functional theory (DFT) calculations also offered a deeper understanding of the extraction mechanism. This study advances the enhancement of battery management with DESs and establishes a validated, quantitative framework that can inspire future innovations in sustainable materials management and contribute to global efforts to support a circular economy in energy storage.

## References

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## Figures

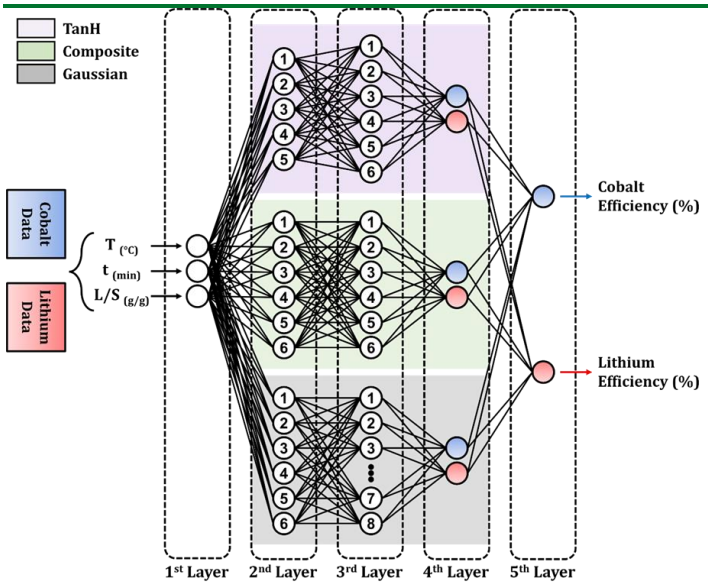


**Figure 1:** Architecture of the ensembled neural network with the hypertuned tanh model (3-5-6-2), composite model (3-6-6-2), GRBF model (3-6-8-2), and the final meta-layer (6-2).

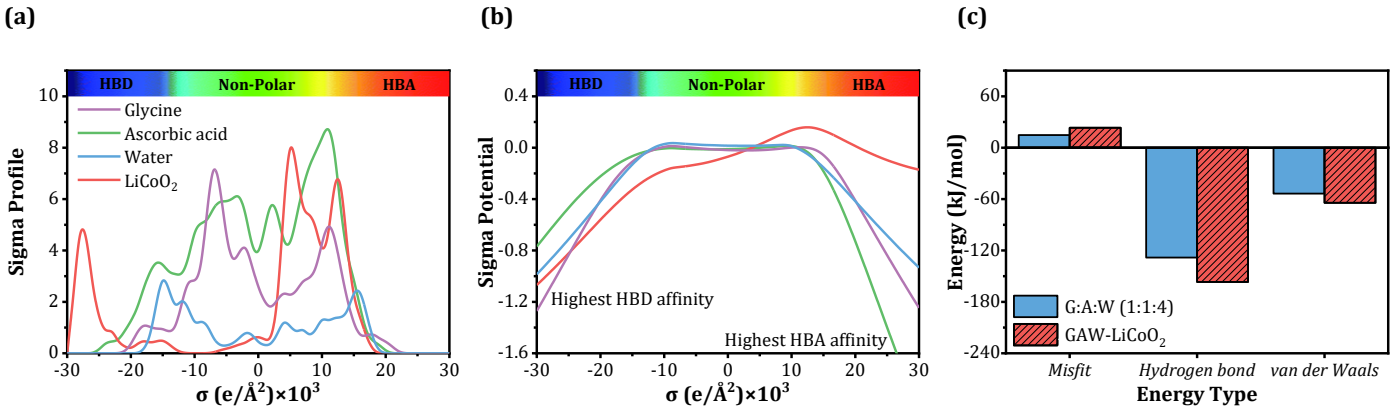


**Figure 2:** Sigma profiles and potentials of individual components in (a) and (b), respectively. (c) Interaction energy distributions of the DES and the complex.