# Integrated Thermodynamic Modelling Approach for the Design of Aqueous Deep Eutectic Solvents for $CO_2$ Capture and Separation at Industrial Conditions

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Among the various alternative solvents that eliminate the drawbacks of traditional aqueous amines, *ad-hoc* designed solvents such as deep eutectic solvents (DESs) emerged as a potential alternative solvent. The potentiality of DESs, in particular as solvents for $CO_2$ capture, is due to the tunability feature of these solvents, wherein the proper selection of the nature and molar ratio of the individual component enables the design of task specific solvent with tailored thermophysical properties for a particular application. However, their high viscosity remains a hurdle to their wide-scale adoption. In this contribution, an integrated modelling approach for the design of aqueous DESs for $CO_2$ capture is developed, combining the predictive power of quantum chemistry calculations using COSMO-RS and a molecular-based equation of state, soft-SAFT, together with thermodynamic modelling. Firstly, the COSMO-RS model is employed to gain molecular-level insight on the intermolecular interactions of aqueous DESs. Subsequently, the soft-SAFT EoS is employed to model the thermodynamic behaviour of aqueous DESs and their $CO_2$ absorption, while examining the effect of water content on $CO_2$ solubility. The model is also employed along with the free-volume theory (FVT) to model the viscosity of aqueous DESs. Lastly, the soft-SAFT model is utilized in a predictive manner to find the optimal water content in DESs that optimizes the solvent performance in terms of $CO_2$ absorption capacity, and viscosity.

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