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Methodology: Chemi-informatics **Oral**

TURNING DEEP-EUTECTIC SOLVENTS INTO VALUE-ADDED PRODUCTS FOR CO_2 CAPTURE

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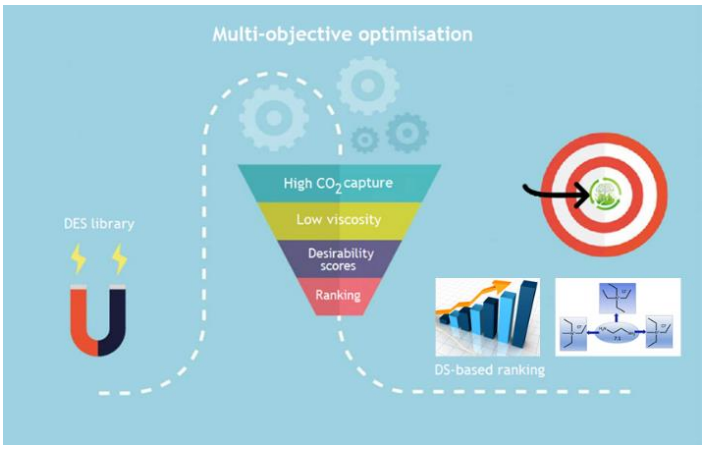
Deep eutectic solvents (DES) are found as promising green solvents for CO_2 capture, especially in large scale industrial applications [1]. Indeed, compared to conventional ionic liquids (IL), DES exhibit similar favourable solvent properties but they are much cheaper, easy to prepare, and more environmentally friendly than IL. However, the major drawback is related to their high viscosity which difficult their management not fulfilling industrial demands. Therefore, additional efforts are needed to develop new DES solvents that possess a greater capacity for CO_2 capture and less viscosity. In this communication, we move a step forward and present results of a practical chemoinformatic approach to simultaneously cope with these two properties. Such approach relies on the application of a multi-objective optimisation (MOOP) technique based on Derringer's desirability function [2]. We began by setting up quantitative structure-property relationship (QSPR) models targeting the two properties for a dataset of known binary DES. Both models were shown to have a very good overall accuracy and predictivity, as well as to provide key information responsible for the DES' higher viscosity and CO_2 capture capacity. Then, the levels of the predictor QSPR variables producing the best possible compromise between both properties were found and applied in a virtual screening (VS) of a hypothetical DES library. In so doing, we were able to rank the top best DES solvents for CO_2 capture earlier to non-effective ones with high probability. Finally, and most importantly, the combined use of the desirability MOOP-based approach and VS proposed here seems to be a valuable chemoinformatic tool for the rational design of novel improved DES solvents for CO_2 capture.



Flowchart showing the desirability MOOP-based chemoinformatic approach and VS ranking

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