Efficient machine learning-based new tools to design eutectic mixtures and predict their viscosity

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In response to the growing demand for sustainable solvents, DES (Deep Eutectic Solvents)[1] have emerged as green alternatives to conventional solvents. However, a major challenge limiting their industrial application lies in their often high viscosity, a property highly influenced by the temperature, the water content, the structure of the components and their ratio in the mixture. Given the vast landscape of possible mixtures, being able to predict the formation and the viscosity of DES has become essential.

To address this, we developed several machine learning models, including classification algorithms able to predict the formation of eutectic mixtures (EM) and regressors that predict their viscosity. The models have been trained on in-house experimental data with several structural descriptors and they have been further validated on sets of unseen data to ensure generalizability and fair extrapolation. In addition, eXplainable Artificial Intelligence (XAI) techniques were employed to quantify input feature contributions to the outputs of the top-performing models.

This talk will begin with a simple introduction to the algorithms and methods used in this study, placing them within the broader context of artificial intelligence (AI) and its applications in chemistry. The main results will then be presented, demonstrating how this study, among others, is a step forward enabling efficient screening of eutectic mixture compositions, tailored for specific applications.

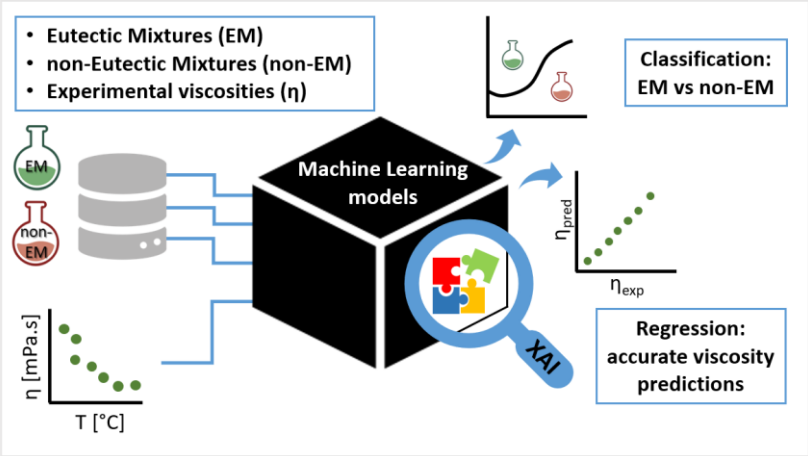

Figure 1: Schematic representation of our machine learning workflow

References

[1] A. P. Abbot et al. Chem. Commun. (2003) **1**, 70-71.