

Artificial intelligence (AI) and machine learning offer tremendous potential to advance materials science and chemical research. AI has the capacity to analyze vast datasets, recognize complex patterns, and make accurate predictions far beyond what is possible for human researchers alone. These capabilities could significantly accelerate the development of new materials with optimized properties for a wide range of applications.

In the chemistry domain, AI is already being applied to enhance various areas of research. For drug discovery and design, machine learning models are being trained to predict the properties and behavior of candidate molecules in order to identify new drug candidates in a more efficient manner. AI is also being used to analyze large datasets of known materials to uncover novel structure-property relationships that can inform the design of new materials with targeted performance.

AI tools show particular promise for accelerating the development of novel functional materials like ionic liquids. These designer solvents are composed entirely of ions and exhibit intriguing properties that make them potentially useful for a broad range of commercial and industrial applications. However, synthesizing ionic liquids with optimized properties for specific tasks remains a challenging trial-and-error process.

Here, model-agnostic meta-learning could offer a powerful approach to predict the sorption capacity of novel ionic liquids more rapidly. By training models on data from related but different sorption tasks, meta-learning aims to extract general patterns that enable a model to quickly and effectively adapt to new tasks with only a small amount of data. This could shift the design of ionic liquids towards a more data-driven paradigm that incorporates prior chemical knowledge to maximize experiment efficiency and discovery velocity.

Model analysis will serve as a foundation for more efficient design of novel task specific ionic liquids which sorption capacity will be assessed during experimental stage of the project for amphotericin and oxygen. Therefore, it will be investigated how this novel algorithm can enhance structural studies on relation between absorption and chemical structural moieties. It is expected that it would be proven that the proposed method can be useful in the structure-property studies even with with low amount of data and the project goal to propose novel task specific ILs with boosted sorption capacity will be reached. Research topic is important for scientific community and was chosen to study in-depth due to rising importance of AI techniques in material science and great importance of ionic liquids in the field of designer green solvents of the future.

In summary, the integration of AI and chemistry has the potential to fundamentally transform how new functional materials like ionic liquids are discovered and developed. With appropriate techniques and datasets, AI tools may enable more rational, data-driven design that accelerates the discovery of ionic liquids tailored for specific high-value applications.