Machine Learning-based approach for Tailor-Made design of ionic Liquids: Application to CO2 capture

유현석, 이용진†
인하대학교
(yongjin.lee@inha.ac.kr†)

This poster presents a machine learning-based approach for the tailor-made design of ionic liquids (ILs) promising toward the desired target applications. Our computational framework combines multi-player Monte Carlo tree search (MP-MCTS) and recurrent neural network (RNN), within a parallel scheme of generating and testing multiple ILs simultaneously, to improve the efficiency of searching optimal structures. For the case studies of CO2 separation from flue gas (CO2/N2) and the separation of from syngas (CO2/H2), target-specific ILs were generated in our computational platform according to objective function values that combine three requirements of high CO2 solubility, absorption selectivity of IL for CO2, and easiness of subsequent desorption. Furthermore, we performed topological data analysis (TDA) on newly designed ILs in materials space and demonstrated that our algorithm can search the material space extensively to find high-performance ILs with good diversity.