A Novel Adversarial Autoencoder With Latent-Based Optimization to Design De-Novo Ionic Liquids for Post-Combustion Carbon Capture

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With atmospheric carbon dioxide concentrations exceeding critical thresholds, the Earth's climate and ecosystems face irreversible damage. To date, the power sector is responsible for 41% of all CO2 emissions; the largest individual contributor by a significant margin. Post-Combustion Carbon Capture (PCC) aims to mitigate this issue by sequestering CO2 from flue gas streams before emission into the atmosphere. Currently, PCC is dominated by amine-based technologies, which suffer various chemical drawbacks that hinder functional and economic efficiency. Ionic Liquids (ILs) have been identified as promising alternative solvents, possessing numerous physicochemical and thermodynamic properties ideal for the process. However, they face a comparatively smaller set of energy and efficiency-based challenges that must be addressed for large-scale implementation to be feasible. It is estimated that there are up to 10^18 unique ILs in the chemical space, yet less than 10^5 have been developed. Exhaustively analyzing such a vast space is computationally impossible. However, the application of current data with deep learning-based techniques can be utilized to yield optimal ILs. In this research, a novel adversarial autoencoder with latent-based optimization was developed. A trained encoder encoded each IL from NIST's database into a low-dimensional latent variable within its latent space. The latent space was trained to follow a viability-based distribution via a discriminator network. Property-optimized latent variables were then converged upon and fed into a trained decoder, resulting in novel, viable, and optimal ILs. The generated structures were deemed significantly superior to existing ILs in terms of targeted properties, and real-world implementation appears promising.

Awards Won:
Association for the Advancement of Artificial Intelligence: Honorable Mention (do not read aloud). Winners receive a student level membership. Information is included separately in the SAO Portal.
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