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"Fantastic Liquids and Where to Find Them: Optimization of Discrete Chemical Space."

Abstract: We present a computational adaptive learning and design strategy for ionic liquids. In this approach we show that (1) multiple cycles of chemical search via genetic algorithm (GA), property calculation with molecular dynamics, and property modeling with physiochemical descriptors and neural networks (QSPR/NN) lead to overall lower property prediction error rates compared to the original QSPR/NN models; (2) chemical similarity and kernel density estimation are a proxy for QSPR/NN error; and (3) single QSPR/NN models projected onto two-dimensional property space recreate the experimentally observed Pareto optimum frontier and, combined with the GA, lead to new structures with properties beyond the frontier.