Closing the loop: Actor-Critic deep reinforcement learning for surface charge density-based solvent design through graph neural networks

Hormazabal Rodrigo[1,2], 양대륙[2,†], 강정원[2]
[1]LG AI Research; [2]고려대학교
(dryang@korea.ac.kr[†])

Solvent selection is a paramount task of chemical process design and drug discovery. With the surge of machine learning research and molecular databases becoming increasingly available, data-driven approaches for solvent design have seen significant improvements. However, databases are heavily concentrated on commonly found structures, which hinder the ability of these models to efficiently improve on yet unknown promising parts of chemical space. In these cases, accurate yet expensive predictions based on quantum calculations are necessary, limiting these design pipelines exploration ability and novelty search. We propose a reinforcement learning approach based on an actor-critic framework, where the actor learns policies on how to modify a molecular scaffold to improve not only the generated structures solvation power but also, how to efficiently refine its own surface density prediction model by generating new training samples through quantum chemical calculations. We explore how this approach compares to widely used deep generative models for molecular design, while also integrating solvation models theory and considering chemical constraints.