Surface charge density prediction for COSMO-based models through distance-aware graph attention neural network

Hormazabal Rodrigo, 강정원, 양대륙†
고려대학교
(dryang@korea.ac.kr†)

Conductor-like screening models (COSMO) have shown great success at quantifying liquid-phase molecular interactions, however, suffer from the extremely time-consuming quantum calculations behind the surface charge density estimations. A graph-based deep learning approach to generate the 3D representation of the polarization surface is presented, which differs greatly from data-driven techniques used to avoid these quantum calculations until now. Previous approaches focus on the prediction of a histogram of the surface charge density, the σ-profile, based on open source databases that contain no more than a few thousand profiles. In this work, the 3D-mesh charge density segments generated by quantum calculations are predicted directly from molecular graphs and basic atom-bond information. Our segment-based method increases the data available to train deep-learning models to the order of millions of examples while allowing for a scalable method that can generalize to bigger compounds. From the whole surface segment prediction, the σ-profile and subsequent calculations can be directly carried on, even for molecular graphs containing more than a hundred atoms.