Predicting the Molecular Electronic Properties by Chemical Knowledge Based Machine Learning Apporach

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Organic fluorescent molecules play the critical roles in the fluorescence inspection, biological probes, and labeling indicators. Learning the design principle of these molecular architectures always attracts the scientific interests of the synthetic and theoretical communities. In this talk, a series of practices of predicting molecular electronic properties will be demonstrated using 10k-plus real world experimental and 100k-plus theoretical datasets, being represented by the chemical knowledge or physical structural information. An assessment of modifying the SchNET models for the predictions of molecular electronic properties, including absorption energy (ΔEabs), emission energy (ΔEemi), and photoluminescence quantum yield (PLQY), is reported. The sample molecules are embedded through the low-dimensional bondstep representation for the purpose of accelerating the dataset preparation. The solution environment is particularly introduced beyond the interaction layers of SchNET. Additionally, the model design principle for the organic molecules prediction are extend to predict the transition metal complexes (TMC) under the conventional framework of Transformer. The predicted HOMO-LUMO gaps of TMCs will be demonstrated.

References

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