Prediction of Intramolecular Reorganization Energy Using Machine Learning

Sule Atahan-Evrenk[a] and F. Betul Atalay[b]

[a] *TOBB University of Economics and Technology, Faculty of Medicine,*
[b] *TOBB University of Economics and Technology, Department of Computer Engineering*
43 Sogutozu Cad. Sogutozu Ankara TURKEY

satahanevrenk@etu.edu.tr

Machine learning techniques offer opportunities for accelerated computational design and discovery. Reorganization energy (RE) is one of the important charge transport parameters suitable for molecular level screening for organic semiconductors. To investigate the possibility of prediction of the RE from the molecular structure by means of machine learning methods, we generated a molecular library of 5631 molecules with extended conjugated backbones. We used benzene, thiophene, furan, pyrrole, pyridine, pyridazine and cyclopentadiene as building blocks for the combinatorial generation of the molecule set and obtained the electronic data at the level of B3LYP level of theory with 6-31G* basis. We compared ridge, kernel ridge, and deep neural net (DNN) regression models based on the graph- and geometry-based descriptors and found that DNN could be used to predict the RE with a mean-absolute-error of 6±10 meV. This study showed that the total RE of organic semiconductor molecules could be predicted from the molecular structure to a high accuracy. We also investigated the possibility of the prediction of the individual contributions of the vibrational modes to the relaxation energy upon ionization.

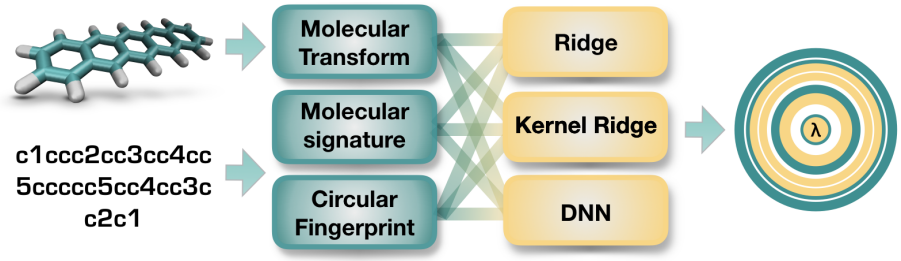

Figure 1: Prediction of the reorganization energy, λ, from molecular structure.