Machine learning for electron-transfer couplings

Chun-I Wang and Chao-Ping Hsu

Institute of Chemistry, Academia Sinica, 128 Section 2 Academia Road, Taipei 115 Taiwan.
cherri@sinica.edu.tw

For developing high-performance organic semiconductors, the understanding of their charge transport behavior is essential. Electronic coupling is a critical factor in determining the charge transfer rates. The values of electronic coupling could be varied by several orders of magnitude even with minor changes in intermolecular configurations. The sensitivity in molecular geometry makes it a critical test with machine learning (ML). In this work, we developed a ML-based approach to predict electronic couplings. We tested kernel ridge regression with the traditional and a simplified Coulomb matrix representation. The ML model trained can successfully reproduce the distance and orientation dependence with a mean absolute error of 3 meV for ethylene dimers. Most importantly, ML model saves 10–1000 times computational cost. With the help of ML, more reliable charge transport dynamics and prediction could be investigated in the future.