Machine learning for fast evaluation of electron-transfer coupling

Chao-Ping Hsu
Institute of Chemistry, Academia Sinica, Taipei, Taiwan 11529
e-mail: cherri@sinica.edu.tw

ABSTRACT

Electron transfer coupling is a critical factor in determining electron transfer rates. It is also the off-diagonal Hamiltonian element when diabatic states are employed in the polaron models. This coupling strength can be sensitive to details in molecular geometries, especially intermolecular configurations. In the charge-transporting dynamics, the effect of such nuclear dependency is the off-diagonal electron-phonon coupling, which has been rarely characterized, possibly due to the large amount of computational resource required in quantum chemistry (QC) calculation. To address this issue, we developed machine learning (ML) approaches to evaluate electronic coupling.[1,2] With these ML models, it becomes possible to investigate the spectral density function of this off-diagonal electron phonon coupling. Here we report such spectral density function and the dynamic implication, together with our recent improvement of Kernel Ridge Regression.

References

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