Electron transfer theory based on diabatic representation

Zhenhua Chen

Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, and College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian 361005, China Zhhchen@xmu.edu.cn

Abstract

In recent years, we developed several *ab initio* quantum chemistry methods to construct diabatic states with specific charge distribution characters and to evaluate the electronic coupling matrix element between the diabatic states at a high-level accuracy. These methods can be applied to study the electron transfer reactions in the diabatic representation.

References

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