
Explicit construction of diabatic state and its application to the direct evaluation of electronic coupling

Zhenhua Chen*, Wei Wu

*Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, and
College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian
361005, China*

* Email: zhchen@xmu.edu.cn

Abstract

In this work, the diabatic states with various localized electron arrangements are explicitly constructed by using nonorthogonal orbital based valence bond theory. Moreover, the electronic coupling, which is the Hamiltonian interaction between diabatic states, is accurately evaluated at the ab initial level.



Zhenhua Chen

