Abstract

We illustrate rate theories for charge transfer and separation in organic molecules for solar cells\(^1\). Starting from the Fermi’s golden rule for the weak electronic coupling, we display the microcanonical and canonical rates, as well as the relationship with Marcus formula. The fluctuation effect of bridges on the rate is further emphasized\(^2\). Then, several rate approaches beyond the perturbation limit are revealed\(^3\). Finally, we discuss the electronic structure theory for the calculations of the electronic coupling and reorganization energy\(^4\) that are two key parameters in charge transfer, and show several applications\(^5\).

Quantum instanton evaluations of the thermal rate constants for complex systems

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Abstract

Quantum instanton (QI) approximation is recently proposed for the evaluation of the chemical reaction rate constants with use of full dimensional potential energy surfaces. Its strategy is to use the instanton mechanism and to approximate time-dependent quantum dynamics to the imaginary time propagation of the quantities of partition function. It thus incorporates the properties of the instanton idea and the quantum effect of partition function, and can be applied to chemical reactions of complex systems. Here, we present the QI approach and its applications to several complex systems dominantly done by us. The concrete systems include: (1) the reaction of \( H + CH_4 \rightarrow H_2 + CH_3 \); (2) the reaction of \( C_2H_6 + H \rightarrow C_2H_5 + H_2 \); (3) H diffusion on Ni(100) surface; and (4) surface-subsurface transport and interior migration for H/Ni. Available experimental and other theoretical data are also presented for a purpose of comparison.