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Theoretical treatment of non-vibrationally-relaxed electron transfer in organic solar cells KUO KAN LIANG, Division of Mechanics, Research Center for Applied Sciences, Academia Sinica, Taiwan, CHIH-KAI LIN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, HUAN-CHENG CHANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan, MICHITOSHI HAYASHI, Center for Condensed Matter Sciences, National Taiwan University, Taiwan, SHENG HSIEN LIN, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — In this work we shall show how to calculate the single vibronic- level electron transfer rate constant, which will be compared with the thermal averaged one. To apply the theoretical results to the dye- sensitized nano-crystalline semiconductor (Grätzel type) solar cells, we use a simple model to describe how we model the final state of the eletron- transfer process (oxidized dye and reduced semiconductor). Numerical calculations of the single-level electron transfer rate constants and the simulation of the quantum beat in the photo-excited state and the product state will be performed to demonstrate the theoretical results.

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