

ROLE OF EXCITON-PHONON COUPLING IN SINGLET FISSION

Zhongkai Huang*, Sayantan Bandyopadhyay[†] and Yang Zhao[‡]

Abstract

Using the Dirac-Frenkel time-dependent variational principle and the multi- D_2 *Ansatz* we have simulated the process of singlet fission. The singlet fission process has seen a resurgence in the recent years because of its ability to bypass the Shockley-Queisser limit of photovoltaics. We have studied the effect of phonon frequencies associated with diagonal and off-diagonal coupling (diagonal and off-diagonal coupling frequencies) and the role of the Huang-Rhys factor. In the case of high off-diagonal coupling frequencies, the efficiency is independent of the Huang-Rhys factor, while in the case of the low off-diagonal coupling frequencies, we obtain a high-efficiency channel. We have further studied the time scales involved in the process for different diagonal and off-diagonal coupling frequencies. We intend to provide a frequency-efficiency analysis to help future development of singlet fission materials.

keywords: Singlet fission, exciton-phonon coupling, singlet-triplet interstate coupling

*Division of Materials Science, Nanyang Technological University, Singapore 639798, Singapore;

[†]Division of Materials Science, Nanyang Technological University, Singapore 639798, Singapore;

[‡]YZhao@ntu.edu.sg; Division of Materials Science, Nanyang Technological University, Singapore 639798, Singapore; Support from the Singapore National Research Foundation through the Competitive Research Programme (CRP) under Project No. NRF-CRP5-2009-04 and from the Singapore Ministry of Education Academic Research Fund Tier 1 (Grant No. RG106/15) are gratefully acknowledged.