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MOLECULAR THEORY OF PHOTOGENERATION

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The elucidation of the time evolution of optically excited states in condensed matter is a fundamental challenge to both a refined scientific probe of materials and to the design of a wide variety of photoelectronic devices. In low mobility materials important aspects of this evolution can be mapped onto a time-dependent random walk (RW) process involving change transfer (CT) steps of an electron and cation between molecular sites. We use this RW process to calculate the dissociation efficiency $\eta(E)$ of these carriers as a function of applied electric field E [1]. The Onsager theory of $\eta(E)$ is formulated in terms of at least two parameters, r_o, the initial separation of the electron-cation pair and η_o the quantum yield for the initial production of the pair. The Onsager approach is shown to be based on an approximation (continuum limit) of the RW process, which is often not valid, especially at small r_o and large E. The emphasis of the talk will be on the importance for $\eta(E)$ of the competition between CT rates and excitation decay rates (R) and how key molecular properties, concentration, temperature, and E affect this competition. The difficulties of interpreting experimental fits for r_o, η_o will be discussed in this context. Detailed features of $\eta(E)$ (including activation energy Δ and high E-saturation) will be illustrated as a function of molecular parameters and system geometry in both the large and small R regimes ($R \rightarrow \infty$ corresponds to the Onsager model boundary condition of an infinite sink at the origin) as well as recent results of a calculation of the slope-to-intercept ratio for this model [2] and a comparison to simulations.

[1] S. Rackovsky and H. Scher, J. Chem. Phys. **89**, 7242 (1988) and references therein.
[2] S. Rackovsky, Chem. Phys. Letters **178**, 19 (1991).