Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information

A charge transfer single crystal field effect transistor operating at low voltages

Abhay A. Sagade,[a] K. Venkata Rao,[b] Subi J. George,[b] Ayan Datta[c] and Giridhar U. Kulkarni[a*]

[a] *Chemistry and Physics of Materials Unit and DST unit on Nanoscience, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Jakkur P.O., Bangalore 560064, India.*
E-mail: kulkarni@jncasr.ac.in

[b] *Supramolecular Chemistry Laboratory, New Chemistry Unit, JNCASR, Jakkur P.O., Bangalore 560064, India.*

[c]*Department of Spectroscopy Indian Association for the Cultivation of Science, Kolkata - 700032, West Bengal, India.*

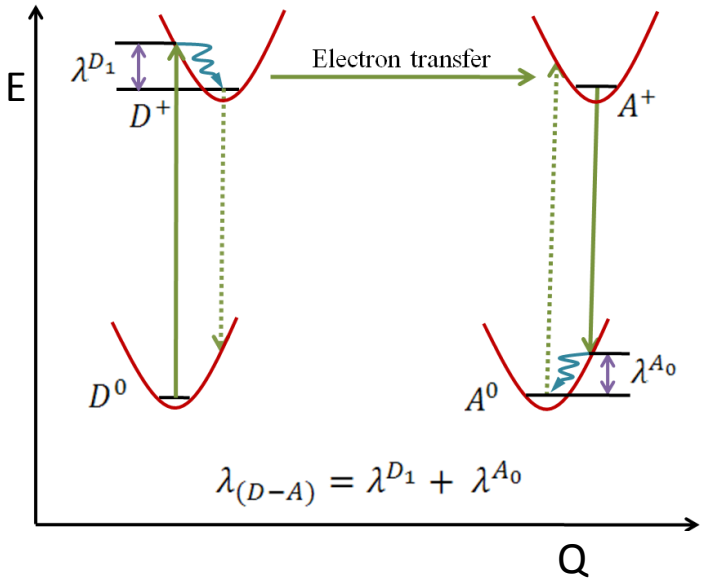

Figure S1. The *E* (relative energy) and *Q* (vibrational reaction coordinates for displacement) representation of the potential energy profile for intermolecular charge transfer in a typical D-A system considered in Marcus Theory. Here, χ is relaxation energy and λ is reorganization energy.

The charge transport mechanism in inorganic semiconductors and organic crystals at low temperature is generally described in terms of the band-model. In this case, strong valence bonds between the different sites delocalize the charges present in the crystal. But for weakly interacting organic crystals, at room temperature, thermal disorder and scattering localizes the charge carriers and the transfer mechanism can be modeled by incoherent hopping of carriers from molecule to the adjacent.[1] In the room temperature limit, the

hopping rate can be described using Marcus theory,[2] $K = (2V^2/h)(\pi^3/\lambda K_B T)^{1/2} e^{-(\lambda/4K_B T)}$ where K_B is the Boltzmann constant and T the temperature. The intermolecular transfer integral (V) and the reorganization energy (λ) are the key parameters which determine the transport efficiency of the material; generally, the former needs to be enhanced and the latter should be minimized for efficient charge transport (Fig. S1).

References

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