

# Electronic structure and conduction mechanism of donor-bridge-acceptor systems where PPV acts as a molecular wire

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p-Phenylenevinylene (PPV) oligomers behave as molecular wires, although in different ways in different experiments. The donor-bridge-acceptor systems [1], where a tetracene donor and a pyromellitimide acceptor are linked by PPV oligomers of varying lengths, have revealed an unusual donor-acceptor distance dependence in the rate constant for photo-induced electron transfer (ET). We have applied density functional theory and other quantum chemical methods to study the electronic structure of PPV-systems and used these data to make conclusions regarding the conduction mechanisms. Consistent with the earlier interpretations we find that the PPV bridges act as a tunneling medium for ET in the thermal case and for the shorter bridges in the photo-induced case. In the longer molecules the photo-induced ET is coherent to the bridge molecule, and is followed by fast draining to the acceptor. Analysis of the electronic structure of the longer bridges allows us to consider these systems as small *molecular wires* providing efficient conduction pathway from D to A.

[1] W.B. Davis, W.A. Svec, M.A. Ratner, M.R. Wasielewski, Nature 396 (1998) 60.

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