**"Understanding Charge transport mechanisms in Organic Materials"**

We present our recent work on the understanding of the charge transport mechanism for organic optoelectronic materials, which has been under controversy. Semiclassical Marcus theory has been extremely popular and insightful for molecular design since Brédas and coworkers [1]. However, the experimental carrier mobility value of organic semiconductors increases rapidly in recent years to well exceed the theoretical limit based on Marcus theory, calling for improvement in computational method beyond the localized semiclassical limit. On the other hand, bandlike transport behavior has been observed for some ultra-pure and closely-packed organic single crystals [2]. We discuss about the effects of charge localization versus delocalization [3], quantum nuclear tunneling [4], dynamic disorder [5], bandlike versus impurity scattering [6], as well as superexchange effect in D-A mixed stacked crystal [7].

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