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Monte Carlo Simulation of Exciton Dynamics in Energy Modulated Heterostructures based on Conjugated Polymer

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Abstract – The main subject of the present work is to demonstrate the use of modulated energy heterostructures to produce efficient directional excitation transfer via Förster processes between PPV segments from the highest HOMO-LUMO gap layer to the lowest band-gap layer. With this concept back-transfer processes can be reduced during energy relaxation between conjugated segments, thus decreasing the probability of the excitation being suppressed by non-radiative processes.

The construction of layered materials which could control the directional migration of the excited state over large distances is still an important subject for both basic and applied physics. In the present work, the step-by-step migration and relaxation processes of the excited state was simulated by Monte Carlo method for different functional heterostructures based on luminescent conjugated polymers. Static and dynamic luminescence, as well as excitation and absorption spectra obtained from simulation were compared with those of real word samples consisting of multiple layered structures prepared with the layer-by-layer technique (LBL) using a poly(p-phenylene vinylene) (PPV) copolymer. Structures with different well- and stair-type energy modulations were prepared and simulated. Simulation of photoluminescence and excitation spectra show that energy gap differences of up to 0.5 eV between the lowest and highest conjugated layers inside the stair structure ware sufficient to guide the excitation over long distances to the lower band gap layer. This result agrees well with experiments. We demonstrated that homotransfer between high energy vibrational states of PPV during the early stages of excitation dynamics accounts for the migration over the structures. These multilayer films having specific supramolecular arrays, controlled at the nanometer level, and the corresponding simulation results can be used to enhance various organic optoelectronic and photovoltaic devices.

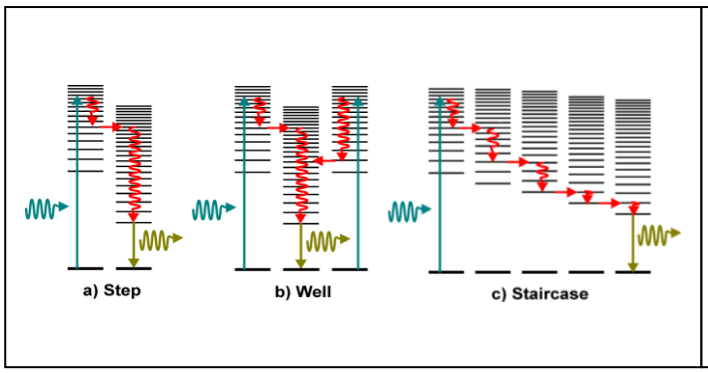

Figure 1: Schemes of graded energy structures used in this work to produce efficient directional excitation transfer process from the highest HOMO-LUMO gap layer to the lowest band-gap layer.

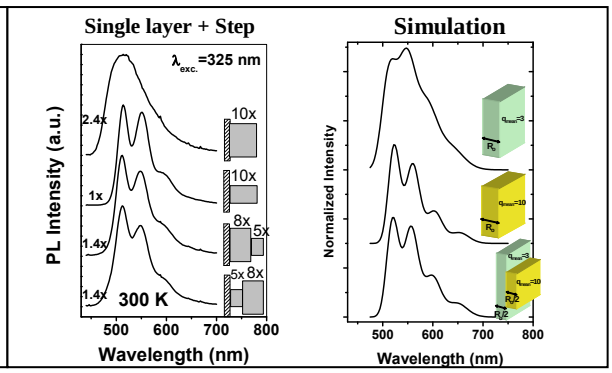

Figure 2: The PLE spectrum of the multiple step structure almost coincides with that of the sample having the lowest HOMO-LUMO gap. This result demonstrates that a small incremental energy steps along the deposition direction provides an effective channel for energy migration inside polymeric layers.