Static and dynamic energetic disorder in OLED materials

Emission layers of organic light-emitting diodes (OLEDs) are composed of emitter molecules dispersed in a host matrix. Relatively low doping concentration prevents detrimental bimolecular processes like triplet-triplet annihilation which lead to non-radiative losses. The role of the host matrix is also to facilitate charge and energy transport as well as to tune optical properties of the emitters. Charge transport (CT) properties of the emission layer govern the rates and pathways of exciton formation. Since the material is an amorphous molecular solid, charges are transported via the hopping mechanism and the mobilities depend on the distribution of CT rates. The overall efficiency of charge recombination depends on the degree of disorder in the material, which can be tuned by the choice of the host matrix.

We use combined molecule dynamics and polarizable QM/MM calculations to investigate energetic disorder in emission layers of OLED materials. To this end we compare ensemble and time distributions of site energies for both, guest and host molecules. The total disorder is partitioned into its static and dynamic components using of the law of total variance. We find that both components are of the same magnitude, but the static component for both guests and hosts is determined by the polarity of host molecules. On the contrary, the dynamic disorder is largely unaffected by intermolecular interactions. The simulations show that the selection of the host component in OLEDs should take into consideration also the amount of static disorder that it introduces in the emission layer.