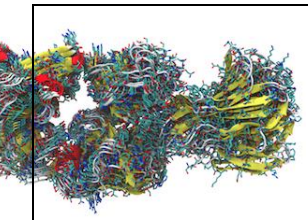

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Emission Redshift in DCM_2-Doped Alq_3: a Non-Linear Stark-Effect Mode

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Abstract:

The basic structure of an Organic Light Emitting Diode (OLED) consists of at least an electron-transporting emissive and a hole-transport layer sandwiched between a cathode and an anode layers, which emits light when an electric current pass through it (electroluminescence). Tris(8-hydroxyquinoline) aluminum(III), Alq_3, is one of the electron transport material and emitting layer most used to date since 1987, when it was first employed. It can also be used with dopants, in order to improve the efficiency of the device.

DCM_2-doped Alq_3 displays a redshift in light-emission frequency which is extremely sensitive to the dopant concentration. This effect can be used to tune the emission frequency in OLEDs.

We can find in literature two models to explain the effect: the solid state solvation effect, proposed by Bulovic *et al.*, and local order theory, proposed by Baldo and Forrest. The first model is based on polarizability difference between the species in organic matrix. Thus, increasing the DCM_2 concentration, increases the strength of the local electric fields present in the film. The second model argues that high electric fields associated with local ordering of polar DCM_2 molecules in aggregate domains contribute to the observed spectral shifts.

In this work, we model the redshift effect using a combination of DFT quantum-chemical calculations and stochastic simulations. We show that the large permanent dipole moments of the DCM_2 molecules generate random electric fields that are large enough to cause a non-linear Stark shift in the band gap of neighboring molecules. As a consequence of this non-linear shifts, a non-Gaussian probability distribution of band gaps for the DCM_2 molecules in the Alq_3 matrix is developed, with long exponential tails to the low-energy side.

We discuss the importance of this distribution, together with the conditions of thermal equilibrium, to explain the experimentally observed emission redshift.