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Determination of the Density-of-States in OLED Host Materials using Thermally Stimulated Luminescence

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Abstract:

Density-of-States (DOS) plays a central role in controlling the charge-carrier transport in amorphous organic semiconductors. The experimental determination of the DOS profile, however, is far from trivial. Several experimental techniques are used to probe the DOS of organic films, such as temperature-dependent space-charge-limited-current spectroscopy, UPS, inverse photoemission spectroscopy, Kelvin probe force microscopy, electrochemically gated transistor approach, as well as thermally stimulated luminescence (TSL). A clear advantage of TSL is that it is a purely optical and electrode-free technique. TSL originates from radiative recombination of charge carriers thermally released from the lower-energy part of the intrinsic DOS that causes charge trapping at very low temperatures.

In this work [1] we apply the low-temperature fractional TSL technique to determine the DOS of pristine amorphous films of organic light-emitting diode (OLED) host materials. The DOS width is determined for two series of hosts, namely, (i) carbazole-biphenyl derivatives: CBP, mCBP, and mCBP-CN, and (ii) carbazole-phenyl derivatives: mCP and mCP-CN. We find that the intrinsic DOS can be approximated by a Gaussian distribution, with a deep exponential tail accompanying this distribution in CBP and mCBP films. The DOS profile broadens with increasing molecular dipole moments, varying from 0 to 6 D, in a similar manner within each series, in line with the dipolar disorder model. This was confirmed by simulations that demonstrate a similar trend in the variation of DOS. The same molecular dipole moment, however, leads to a broader DOS of CP compared with CBP derivatives. Using QM/MM Molecular Dynamics simulations, it was attributed the difference between the series to a smaller polarizability of cations in CP derivatives, leading to weaker screening of the electrostatic disorder by induction. These results demonstrate that the low-temperature TSL technique can be used as an efficient experimental tool for probing the DOS in small-molecule OLED materials.

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References:

[1] A. Stankevych, A. Vakhnin, D. Andrienko, L. Paterson, J. Genoe, I. I. Fishchuk, H. Bässler, A. Köhler, A. Kadashchuk, Density of States of OLED Host Materials from Thermally Stimulated Luminescence, Phys. Rev. Applied. 15, 044050 (2021).