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

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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 SCLC, UPS, inverse photoemission spectroscopy, Kelvin probe force microscopy, as well as thermally stimulated luminescence (TSL). A clear advantage of TSL is that it is a purely optical and electrode-free technique.

In this work we apply the low-temperature fractional TSL technique to determine the DOS of pristine amorphous films of 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. The DOS profile broadens with increasing molecular dipole moments, in a similar manner within each series, in line with the dipolar disorder model. The same molecular dipole moment, however, leads to a broader DOS of CP compared with CBP derivatives. Using QM/MM Molecular Dynamics simulations, we attribute 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 can be used as an efficient experimental tool for probing the DOS in OLED materials.

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1. A. Stankevych, A. Vakhnin, D. Andrienko, L. Paterson, J. Genoe, I. I. Fishchuk, H. Bässler, A. Köhler, A. Kadashchuk, Phys. Rev. Applied. (2021), 15, 044050.