Fused Quinoidal Oligothiophenes Imides with High Electrical Conductivity

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Organic diradicals are molecules containing two unpaired electrons, which are usually highly reactive.[1-2] Although these organic diradicals present a wide range of potential applications, their air stability still remains as a major obstacle.[3] In order to overcome this, new organic diradicals based on quinoidal oligothiophenes-derivatives (QOT) have been synthesized, *i.e*. BTICN, ISOCN and QTICN (see Figure 1). These new molecules present high stability and electrical conductivity, which have been achieved by employing imide-bridged fused molecular frameworks. The combination of strong electron-withdrawing imide with tetracyano groups in the conjugated skeletons also enabled extremely deeply aligned LUMO levels and large diradical character assisted by cross-conjugation.[4]
Here we use different experimental techniques and DFT calculations to provide new insights into the electron conduction mechanism of QOT diradicaloids, in order to demonstrate the great potential of fused quinoidal oligothiophene imides in developing stable organic diradicals and high-performance doping-free n-type conductive materials.

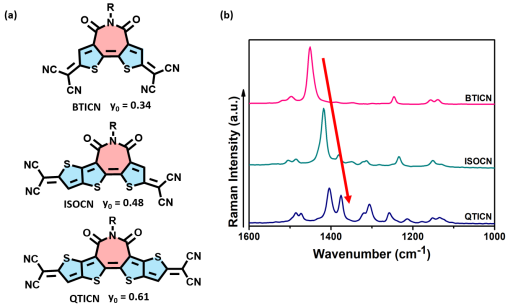

Figure 1. a) Chemical structures and b) FT-Raman spectra of quinoidal systems BTICN, ISOCN and QTICN studied in this work.

References

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