SPIC 2022 : Quatrième congrès national Sciences et Technologies des systèmes pi-conjugués
5-8 déc. 2022, Saint Malo 35407 (France)

Elusive killer phonons in herringbone-packed molecular semiconductors

Nemo McIntosh[1,*], Claudio Melis[2], Samuele Gianini[1], Federico Modesti[3], Vincent Lemaur[1], Yves Geerts[4], Peter Erk[3], Luciano Colombo[2], David Beljonne[1], Jérôme Cornil[1]

[1] *Laboratoire de Chimie des Matériaux Nouveaux, Université de Mons, Mons, Belgique*
[2] *Physics Department, University of Cagliari, Cagliari, Italy*
[3] *BASF SE, Ludwigshafen am Rhein, Germany*
[4] *Laboratory of Polymer Chemistry, Université Libre de Bruxelles, Bruxelles, Belgique*
* nemo.mcintosh@umons.ac.be

We present a method to quantify the effect phonons have on the fluctuation of the transfer integrals (a measure of charge delocalization between two molecules), and thus how they affect charge mobility in devices. We compare two thienoacene molecules that comprise two and four central tetrathienyl cores fused with naphtyl rings, DNTT[1] and DN4T[2] respectively. The two molecules are very similar on many aspects; they display high electron density on their sulfur atoms resulting in rather high transfer integrals, pack in the same fashion and have practically the same unit cell dimensions. Both materials lie in the typical grey area between hopping and band-like mobility.

The carrier mobility in these crystals is known to be limited by low-frequency phonons collapsing the wavefunction at room temperature. Remarkably, we find that the transfer integrals in DN4T are rather insensitive to the sliding motion of the aromatic cores, reported to be the 'killer' mode in DNTT and C8-DNTT-C8[3]. We computed the electron-phonon coupling spectra for several cell sizes which allow us to assess the vibrational modes governing the extent of the fluctuations and the role of phonon dispersion.

References

[1] Kang MJ et al. Advanced Materials 23.10 (2011): 1222-1225.
[2] Jouclas R. et al. Advanced Science (2022): 2105674
[3] Schweicher G. et al. Advanced Materials 31.43 (2019): 1902407

Acknowledgement

This project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 811284 (UHMob)