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Mechanism of conductivity in high-mobile organic semiconductors using THz spectroscopy

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Organic molecular crystals with high mobility have recently emerged as promising candidates for field-effect transistor applications. Among them, DNTT (dinaphtho[2,3-b:2′,3′-f]thieno[3,2-b]-thiophene) and its alkylated derivative, C8-DNTT-C8, have been shown to exhibit some of the best-performing organic semiconducting properties, with experimental field-effect transistor charge carrier mobilities reaching up to 8-11 $cm^2 V^{-1} s^{-1}$.

However, describing charge carriers in molecular semiconductors using Bloch wavefunctions is not possible due to their small electronic mean free path relative to the intermolecular distance. Instead, charge transport in these materials is believed to occur through incoherent hopping between states confined to individual molecules. This process is thought to be thermally activated, leading to an increase in mobility with temperature in line with classical Marcus theory. Nonetheless, some studies have reported a weak power-law decay of mobility with temperature, which has raised questions about the true charge transport mechanism in OSs.

In this work, we present a contact-free measurement of the temperature-dependent mobility of DNTT and C8-DNTT-C8 using THz spectroscopy. By combining our experimental results with atomistic fragment orbital-based surface hopping (FOB-SH) theory, we provide a comprehensive description of charge transport in these two high-mobility OSs. Our study highlights the profound impact of small changes in chemical structure on the temperature-dependent behavior of charge carriers in OSs.

Biography

She obtained her master's degree in Physics with a specialization in Condensed Matter Physics from the University of Pisa. Currently, she is working as a Ph.D. student at the Max Planck Institute for Polymer Research in the UHMob Project, which is a part of the multi-site European Training Network (ETN) running from 2019 to 2023, funded by the EU FP - Horizon 2020, Marie Skłodowska-Curie Actions. Under the supervision of Professor Mischa Bonn, her research focuses on investigating the mechanism and efficiency of conductivity in high-mobility organic semiconductors using Terahertz spectroscopy.

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