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Temperature activated transport tuned by libration in the charge-transfer salt trans-stilbene – 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (STB-F_4TCNQ) KATELYN P. GOETZ, Wake Forest University, DEREK VERMEULEN, University of North Carolina at Chapel Hill, MARGARET E. PAYNE, WFU, JIANG HUI, HU PENG, Nanyang Technological University, CYNTHIA S. DAY, WFU, CHRISTIAN KLOC, NTU, VEACESLAV COROPCEANU, Georgia Institute of Technology, LAURIE E. MCNEIL, UNC, OANA D. JURCHESCU, WFU — A common route to solubility in organic semiconductors is chemical functionalization. This adds librational modes to the molecules, which was theoretically predicted to impact charge transport. We discuss the effect of libration on charge transport in the charge-transfer complex trans-stilbene–2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (STB-F_4TCNQ). This material has a 300 K mobility of 0.3 $cm^2V^{-1}s^{-1}$ that decreases with an activation energy of 170 meV to 235 K, where it transitions to temperature independence. X-ray diffraction indicates that the cause of this is the freezing of the libration of the ethylene moiety within STB below 235 K. Above 235 K, it increases in amplitude with increasing temperature. Fourier difference maps suggest that the charge density unaccounted for by the STB and F_4TCNQ molecules is localized on the molecules at low temperature and more delocalized after the transition. This agrees with XRD and Raman spectroscopy estimates for the degree of the ground state donor to acceptor charge transfer, indicating zero transfer below and 0.1 electrons above the transition temperature, highlighting the strong coupling between molecular motion and charge transport.

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