

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Charge Transport in Functionalized Fluorinated Pentacenes

OANA JURCHESCU, DANIEL DAVID, CLAIRE MCLELLAN, Wake Forest University, BALAJI PURUSHOTHAMAN, University of Kentucky, SHUBIN LIU, University of North Carolina, VEACESLAV COROPCEANU, Georgia Institute of Technology, JOHN ANTHONY, University of Kentucky, LAURIE MCNEIL, University of North Carolina — We report on charge transport in fluorinated functionalized pentacenes and discuss the effect of trialkylsilyl and the number of fluorine atoms. We show that modifications in the chemical composition influence the molecular packing, crystal formation and electrical properties, allowing us to measure mobilities from 10^{-5} to $1.7 \text{ cm}^2/\text{Vs}$. The mobilities correlate with the packing, demonstrating that tuning the solid-state order to induce pi-stacking improves electrical properties. By combining Raman measurements with theoretical calculations predicting the vibrational spectrum, we explore the vibrational modes of the crystals, providing information about the intermolecular coupling and electron-phonon interactions governing charge transport. We calculate the intermolecular electronic couplings and band structures by using density functional theory, and study the effect of fluorination and trialkylsilyl substitution on crystal packing and the electronic properties.

Oana Jurchescu
Wake Forest University

Date submitted: 18 Nov 2010

Electronic form version 1.4