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**Effects of -$NO_2$ substitution on charge addition and reorganization energies in phenylene ethynylene oligomers** STEVEN ROBEY, NIST-Gaithersburg, N. E. GRUHN, University of Arizona, J. CIZEK, Rice University, J. M. TOUR, Roice University — Reports of non-linear transport in molecular-scale junctions have stimulated suggestions for computing and switching applications based on molecular electronics. One of the most widely referenced results is reported negative differential resistance (NDR) behavior in -$NO_2$ substituted oligo- phenylene ethynylenes (OPE). Theoretical work has invoked the importance of charge addition effects on conformation and electronic structure and polaronic effects to provide potential explanations for this behavior. We have investigated charge addition effects for pristine versus -$NO_2$ substituted OPE self-assembled monolayers using photoelectron spectroscopy in combination with "doping" with K. Results are consistent with differences arising from filling of levels associated with the - $NO_2$ group. We have investigated polaronic effects using photoelectron spectroscopy and optical absorption to guide calculations of reorganization energies for pristine versus -$NO_2$ substituted OPE's. We find theoretical evidence for increased reorganization energy with -$NO_2$ substitution for anionic species by about 33 percent, with experimental values of the reorganization energy ranging from about 0.2 eV to 0.4 eV and theoretical values about 0.2 eV.

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