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**Charge addition effects in phenylene ethynylene oligomers: the effect of -NO<sub>2</sub> substitution** S. W. ROBEY, C. D. ZANGMEISTER, R. D. VAN ZEE, NIST-Gaithersburg — Interest in aromatic systems based on phenylene ethynylene oligomers (OPE) has been spurred by reports of interesting negative differential resistance/hysteretic behavior in metal-molecule-metal junctions. 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 the influence of charge addition, via “doping” with K, in pristine versus nitro-substituted OPE using photoelectron spectroscopies. Sequential addition of K in unsubstituted OPE produces a gradual shift to higher binding energy, reminiscent of “rigid band” behavior, with relative shifts of  $\pi$  levels suggesting some distortion/conformation change. For a nitro-substituted oligomer, a markedly different behavior is observed with K addition. After an initial shift, the electronic levels are pinned for subsequent K addition before a final shift brings the spectrum to near coincidence with that for the pristine oligomer. Potential explanations for this behavior are provided based on model calculations of the effects of charge addition on the molecular electronic structure. We have also investigated differences in the reorganization energy that accompanies charge addition/removal in these systems by a combination of photoelectron and optical spectroscopies and theoretical calculation.

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