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Photoelectron Spectroscopy as a Probe of Molecular Clusters Relevant to Singlet Fission STEVEN KREGEL, GLEN THURSTON, ETIENNE GARAND, University of Wisconsin-Madison — The singlet fission (SF) process has recently become of great interest to the physical chemistry community due to its potential application to next-generation solar cells. The relative energetics of the singlet and triplet states involved in this process are of fundamental importance to SF, as is the magnitude of the inter-chromophore coupling. Due to this coupling, the electronic structure of small chromophore clusters is different from the bulk, as well as from isolated molecules. In order to study these systems we have constructed a new instrument consisting of a time of flight mass spectrometer coupled to a high resolution photoelectron spectrometer. Utilizing this instrument, we are able to generate small chromophore clusters (n=1-5) of known mass, and interrogate them individually with sensitivity to both singlet and triplet excited states. By utilizing anion photoelectron spectroscopy we can map out the energy landscape of the final neutral systems as a function of cluster size, while simultaneously directly measuring the magnitude of electronic coupling between individual chromophores. Preliminary studies with this instrument have focused on anthracene and tetracene which have been shown to exhibit SF in crystals, along with similar polyaromatic hydrocarbons.

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