CAN FEMTOSECOND TRANSIENT ABSORPTION SPECTROSCOPY PREDICT THE POTENTIAL OF SMALL MOLECULES AS PERSPECTIVE DONORS FOR ORGANIC PHOTOVOLTAICS?

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The utility of a perspective donor or acceptor molecule for photoelectric applications is difficult to predict a priori. This hinders productive synthetic exploration and necessitates lengthy device optimization procedures for reasonable estimation of said molecule's applicability. Using femtosecond broadband transient absorption spectroscopy, supported by time-dependent density functional theory computations and steady-state-absorption and emission spectroscopies, we have characterized a family of perspective optoelectronic compounds, in an effort to predict their relative performance in organic photovoltaic devices from information accrued from excited-state dynamics and photophysical properties.

A series of tetraphenylazadipyrromethene (ADP) complexes chelated with three different metal centers was investigated. We have determined that the chelating metal has little effect on the ground state properties of this family. However their excited state dynamics are strongly modulated by the metal. Specifically, the zinc-chelated ADP complex remains in the excited state tenfold longer than the cobalt or nickel complexes. We assert that this is key photophysical property that should make the zinc complex outperform the other two complexes in photovoltaic applications. This hypothesis is supported by preliminary power conversion efficiency results in devices.