Rational Design and Synthesis of Small Molecule Based Materials for Solar Cell and Photodynamic Therapy Applications: Organic small molecule based materials offer great promise in technologies such as solar cells and photodynamic therapy, due to their versatility and low-cost. However, to make them commercially viable, some challenges still remain. For instance, the current small molecule based solar cells are still quire inefficient compared to inorganic materials. A significant, fundamental difference between these materials is the mechanism for the formation of excitons upon absorption of photons. Inorganic materials, such as silicon based materials, generate Wannier excitons while organic materials generate Frenkel (molecular) excitons. Current studies indicate that materials that produce the Wannier excitons are superior in devices such as solar cells. Therefore, our objective in this research is to understand the

excitons being generated in organic small molecules (e.g., Fig.1) tuning exciton energies and design new materials that can generate Wannier excitons.

Using commercially available software and our in-house generated code, we will study a series of small organic molecule based materials and use those cases to design new materials. We will also design small molecule based materials and use those cases to design using the degeneracy concept that was recently developed in our group to generate Wannier excitons. The predicted materials will then be synthesized and characterized for their performance in solar



Fig. 1. Functional groups used to tune optical properties of 4-vinyl-N,N-di(p-tolyl)aniline (MTPA) and the molecules to be designed.

cells and photodynamic therapy applications. The REU students will learn how to computationally design molecules and predict their properties (in Wang group) and then synthesize the molecules in the laboratory (in Plunkett group). In this project, the **REU students** will perform computations to obtain the optical properties of various candidate molecules and design the synthesis of new materials based on the results. The REU students will experience the process of computationally assisted rational design of materials for various applications such as in energy and medicinal applications.

More information on the proposed research and related publications can be found in the groups' website. Wang group: <u>http://chem.siu.edu/faculty-staff/faculty/wang.php</u>; Plunkett group: <u>http://chem.siu.edu/faculty-staff/faculty/plunkett.php</u>.