## Dantus Research Group Research Interests

## Super Photo-Reagent Discovery and Characterization



Our group, in collaboration with other world-wide experts is seeking to find compounds able to harness the energy of photons to achieve outstanding chemical reactivity. Starting from  $\Delta G = RT \ln K$ , our goal is to find high energy configurations (excited states) that are long lived and have much greater  $\Delta G$ . We recently published on the world's first super photobase, a compound that goes from a pK<sub>a</sub> ~ 7 in the ground state to a pK<sub>a</sub> ~ 21 in the excited state. See for example: Angew. Chem. Int. Ed. <u>57</u>, 14742 –14746 (2018).

Progress in this area requires spectroscopic characterization of multiple materials. We use a number of spectrometers capable of determining both the equilibrium and the transient linear and nonlinear (femtosecond, picosecond, nanosecond) spectroscopic behavior of this materials. This work is presently funded by the National Science Foundation.



## Femtosecond Triggered High-Energy Chemistry

When an intense laser interacts with an isolated molecule the laser field is able to pull an electron and ionize the molecule. In some cases, the electron is accelerated by the field and it recollides with the molecule setting off high-energy chemical reactions. Our group is studying such high-energy reactions, for example: for methanol we find CH<sub>3</sub>OH yields  $H_3^+$  and HCO<sup>+</sup> after such excitation. The reaction occurs in 100 fs. It starts by double ionization of the oxygen atom; this is followed by formation of neutral  $H_2$  which roams and extracts a proton to form  $H_3^+$ . This type of chemistry has never been explored and is highly relevant to astrochemistry. *See for example: J. Chem. Phys.* <u>150</u>, 044303 (2019); *Nat. Commun.* <u>9</u>, 5186 (2018); *Nat. Sci. Rep.* <u>7</u>, 4703 (2017). This work is presently funded by the Department of Energy. More recently we are learning to control these processes by controlling the electron acceleration step.