

# Computational Chemistry: What is it Good For?

(Absolute everything. Say it again)\*

The interpretation of modern experimental measurements and syntheses in chemistry is greatly aided through a variety of sophisticated computational chemistry techniques (in particular ab initio electronic structure methods). These methods can be used for determining molecular geometries, bonding (electronic structure), and physical as well as photophysical properties of molecules. Computational chemistry can go beyond simply interpreting existing experiments to the prediction of new species with novel properties. In this talk, I will highlight recent examples from our work on phosphorescent tellurophene-compounds and molecular precursors for materials chemistry (research in collaboration with Prof. E. Rivard, University of Alberta). I will then move from materials chemistry research to chemical biology to discuss the design of fluorescent proteins with strong two-photon absorptions for biological imaging. From these examples, I will showcase the strong role computational chemistry plays in modern chemistry research.

\* with apologies to N. Whitfield, B. Strong and their song “War” recorded E. Starr (1970)

