

# Controlling Chemistry with Light and Force

Todd J. Martínez

Department of Chemistry, Stanford University

A major goal of chemistry is understanding how external influences can be used to control molecular transformations. We introduce the *ab initio* multiple spawning (AIMS) method as a means of calculating the behavior of molecules exposed to light or external forces (photochemistry and mechanochemistry). We then discuss photoinduced *cis-trans* isomerization reactions in isolated, solvated and protein environments and describe a simple picture for predicting the outcome of these reactions, e.g. which bond isomerizes in molecules with multiple isomerizable bonds and whether the molecule isomerizes or fluoresces. The implications for photobiological systems like the Green Fluorescent Protein (GFP) and Photoactive Yellow Protein (PYP) are elucidated. We then discuss an alternative means of controlling molecular behavior, namely the use of external forces. A few applications are presented, including mechanochromic polymers. We highlight the parallels between photochemistry and mechanochemistry and speculate about the possibility of designing molecules which are both photo- and mechano-sensitive.