

Computational Design of Dyes for Bioimaging: Semiempirical Approaches

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This talk will begin with an overview of semiempirical quantum chemical methods, including their uses and limitations. The application of these methods to the design of dyes for bioimaging applications will then be discussed. One of the goals is to design dyes that fluoresce only when bound to a protein, so that the location of multiple proteins can be tracked in a living cell with a fluorescence microscope. Another goal is to design dyes whose fluorescence changes in the presence of Na or K ions, so that the transmission of signals along a neuron can be imaged in real time. In both cases, semiempirical computations have helped show how the protein or ion alters the fluorescence of the dye, and led to suggestions for improving the dye's sensitivity. The talk will close with an overview of a new project in which computer scientists and chemists are collaborating to use methods from machine learning to develop new semiempirical models.