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Using computational chemistry to understand proton transfer in Green Fluorescent Protein[1] CHRISTA HOSKIN, PAUL CHAMPION, TIMOTHY SAGE, ABDELKRIM BENABBAS, ALEXANDER DEMIDOV, BRIDGET SALNA, Northeastern University, JASPER VAN THOR COLLABORATION[2], LEE THOMPSON COLLABORATION[3] — Green Fluorescent Protein has been studied experimentally by the scientific community for years yet frustratingly little is known about the underlying proton transfer process that produces the green fluorescence. We are trying to elucidate more about this process using Density Functional Theory to prepare and run various calculations on GFP that we compare with kinetics data, Raman and vibrational coherence spectra. I am building a model of wild type GFP that is realistically sized for our computational power, yet still contains key residues that might affect the proton transport process. I will compare my results to those of the E222D GFP mutant. This comparison will allow us to see any differences in energy and normal modes that give insights regarding the proton transfer process. For example, how does it depend on a variety of factors such as temperature, buffer, pH, mutations, etc.? We also plan to examine if the proton transfer propagates through the three donor-acceptor pairs of the "proton wire" consecutively versus the three protons on the wire transferring simultaneously. Finally, we will consider how quantum tunneling may be involved in the proton transfer.

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