Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Structure and Spectra in Mutated Green Fluorescent Protein: A Combined Molecular Dynamics and QM/MM Study SOUMYA PATNAIK, STEVEN TROHALAKI, RUTH PACHTER, Air Force Research Laboratory — Recently, several Green Fluorescent Protein (GFP) mutants have been developed with red-shifted absorptions. The molecular structures of two such mutants with S65G and S65T mutations have been studied with an aim towards understanding the shift in their absorption spectra. A combined approach of molecular dynamics (MD) and Quantum Mechanics/Molecular Mechanics (QM/MM) has been used. Time dependent density functional theory (TDDFT) based absorption spectra calculations were found to be of excellent agreement with experimental data. These calculations were carried out on chromophore structures derived from QM/MM and MD studies, thus taking into account, both the effects of thermal fluctuations and the protein and solvent environment. In addition to providing information regarding the variation of the geometrical parameters due to temperature effects, the MD simulations also identify residues around the chromophore which are associated with conformational change on mutation. By using QM/MM to systematically analyze significant structural features that were identified by MD simulations, a detailed understanding of the energetics of the optimized chromophore conformations was achieved.

Soumya Patnaik
Air Force Research Laboratory

Date submitted: 07 Dec 2005 Electronic form version 1.4