Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Molecular dynamics simulation studies of dielectric response and vibrational energy relaxation in photoactive yellow protein and green fluorescent protein YAO XU, RAMACHANDRAN GNANASEKARAN, DAVID LEITNER, University of Nevada, Reno — The first step in the photocycle of many proteins involves conformational change of a chromophore or a charge transfer reaction following photoexcitation. To explore the response of the protein and solvent environment to photoexcitation of the chromophore in photoactive yellow protein (PYP) and green fluorescent protein (GFP) we carried out molecular dynamics simulations of the dielectric response and vibrational energy relaxation (VER) from the chromophore to the protein and solvent. In PYP the time scale of the protein response, mainly contributed by Tyr42 and Glu46, to photoexcitation appears prominently between 0.1 and 0.3 picoseconds. The frequency-dependent VER rate also reveals dynamic coupling between the chromophore and residues that hydrogen bond to it. Resonances in the VER rate appear at frequencies comparable to the oscillations observed in recent fluorescence decay studies. In GFP, which undergoes excited state proton transfer about 10 ps following photoexcitation that may be assisted by specific chromophore vibrations, both the protein and water molecules inside the β-barrel surrounding the chromophore mediate the dielectric response.

Yao Xu
University of Nevada, Reno

Date submitted: 14 Nov 2011 Electronic form version 1.4