Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Dissecting the active site of a photoreceptor protein WOUTER HOFF, MIWA HARA, JIE REN, FARZANEH MOGHADAM, AIHUA XIE, MASATO KUMAUCHI, Oklahoma State University — While enzymes are quite large molecules, functionally important chemical events are often limited to a small region of the protein: the active site. The physical and chemical properties of residues at such active sites are often strongly altered compared to the same groups dissolved in water. Understanding such effects is important for unraveling the mechanisms underlying protein function and for protein engineering, but has proven challenging. Here we report on our ongoing efforts on using photoactive yellow protein (PYP), a bacterial photoreceptor, as a model system for such effects. We will report on the following questions: How many residues affect active site properties? Are these residues in direct physical contact with the active site? Can functionally important residues be recognized in the crystal structure of a protein? What structural resolution is needed to understand active sites? What spectroscopic techniques are most informative? Which weak interactions dominate active site properties?

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Date submitted: 08 Nov 2015 Electronic form version 1.4