

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Diffusion of molecular oxygen in the red fluorescent protein mCherry¹ CHOLA REGMI, YUBA BHANDARI, BERNARD GERSTMAN, PREM CHAPAGAIN, Florida International University — The monomeric variants of red fluorescent proteins (RFPs), known as mFruits, have been especially valuable for tagging and tracking cellular processes *in vivo*. Determining the oxygen diffusion pathways in FPs can be important for improving photostability and for understanding maturation of the chromophore. We use molecular dynamics (MD) calculations to investigate the diffusion of molecular oxygen in one of the most useful monomeric RFPs, mCherry. We investigate a pathway that allows oxygen molecules to enter from the solvent and travel through the protein barrel to the chromophore. The pathway contains several oxygen hosting pockets, which are identified by the amino acid residues that form the pocket. The results provide a better understanding of the mechanism of molecular oxygen access into the fully folded mCherry protein barrel and provide insight into the one of the photobleaching processes in this protein.

¹Work supported by NIH/NIGMS grant SC3-GM096903.

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Date submitted: 12 Nov 2012

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