

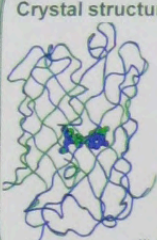
Primary Events of Photodynamics of GFP Chromophore in Different Environments

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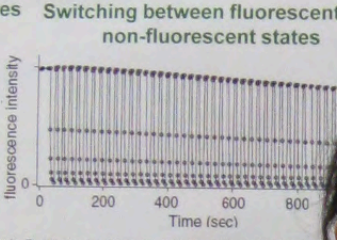
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Crystal structures



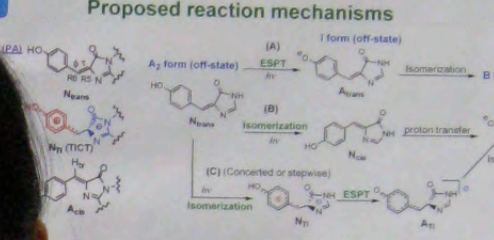
Switching between fluorescent and non-fluorescent states



(1) Ando, R.; Mizuno, H.; Miyawaki, A. *Science* 2004, 306, 1370. (2) Ando, R.; Trowitzsch, S.; Weber, G.; Egeling, C.; Wahl, M. C.; Hell, S. W. *Science* 2005, 307, 1131.

Background

Proposed reaction mechanisms



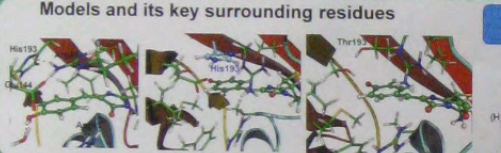
(A) A_2 form (off-state) \xrightarrow{ESPT} I form (off-state) $\xrightarrow{isomerization}$ B form (on-state)

(B) A_2 form (off-state) $\xrightarrow{isomerization}$ I form (off-state) $\xrightarrow{proton transfer}$ B form (on-state)

(C) (Concerted or stepwise) A_2 form (off-state) $\xrightarrow{isomerization}$ I form (off-state) \xrightarrow{ESPT} B form (on-state)

(*) Ando, R.; Mizuno, H.; Miyawaki, A.; Morokuma, K. *J. Phys. Chem. B* 2010, 114, 1114.

Models and its key surrounding residues

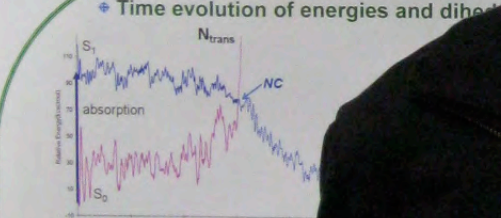


His193, His194, Thr192

Model Systems

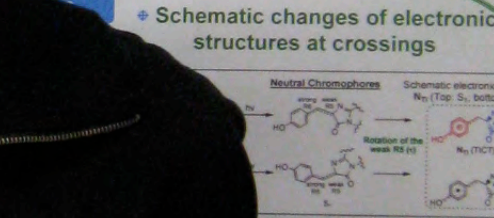
Methods:
 Non-adiabatic ONIOM(QM:MM) MD;
 QM: SA2-CASSCF; MM: Amber96
 Laudau-Zener model
 Gaussian Development Version, Molpro, Modified Tinker
 (PDB IDs: 2IOV and 2POX)

Time evolution of energies and dihedral angles



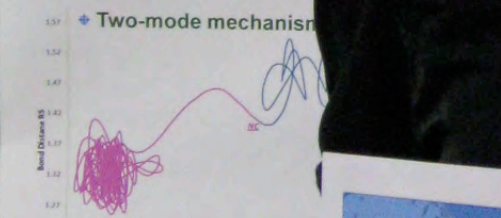
absorption, S_1 , N_{trans} , N_C , S_0

Schematic changes of electronic structures at crossings




Neutral Chromophores, Schematic electronic states of N_{T1} (Top: S_1 , bottom: S_0)

Two-mode mechanism



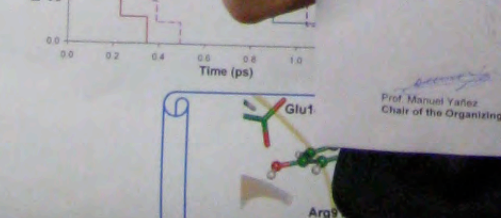
Bead Distance (Å)

Excited-state population




Excited-state population, Time (ps)

Excited-state population

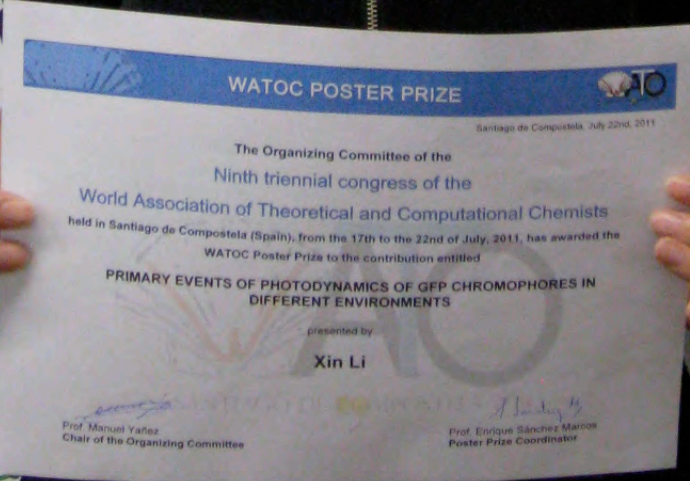


Dihedral angle (194), Excited-state population, Time (ps)

Excited-state population



Excited-state population, Time (ps)



X. Li, L. W. Chung, H. Mizuno, A. Miyawaki, K. Morokuma. *J. Phys. Chem. Lett.* 2010, 1, 3328.

Presentations
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