Multi–Scale Modeling of Proteins

Supporting Information

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Table 1: Selected theoretical calculations of the excitation energies of the GFP chromophore. The calculation in a solvated environment are performed either with microsolvation or with continuous polarizable models.

	neutral	in water	anion	in water
semiempirical				
INDO-CI *a,b*	3.81		2.77	2.85
NDDO-G-CI *c*	3.47		2.70	
NDDO-OM2/PERTCI *d*	3.44		2.48	
MNDOC-CASCI *e*	3.52		2.70	
AM1-CASCI *f*	3.56			
AM1-CISD *f*	3.83			
PM3-CASCI *f*	3.51			
MNDO-CASCI *f*	3.84			
AM1-FOMO-CI *g*	3.58	3.52		
ab initio				
HF *h*	5.53		4.71	
UHF *h*	3.51		2.29	
CIFS *h*	5.23		4.37	
MSCF *h*	4.52		3.54	
SAC/SAC-CI *i*	3.33		2.22	
CASSCF *j*	5.25			
CASPT2 *j,k,l,m,n*	3.85 3.69 3.56		2.67 2.66	2.85
TDDFT				
BLYP-TD *n*	3.33		3.24	
B3LYP *n,j,o*	3.54 3.46	3.30	3.08 3.07	2.97
B3LYP+corr *n*	3.52		2.65	
BPE-TD *p*	3.57	3.38	3.12	3.02
Expt *q,r,s*		3.33 3.31 3.29	2.59	2.92

Acronyms: INDO, NDDO, AM1, PM3 = different kinds of semi-empirical Hamiltonians; (U)HF = (Unrestricted) Hartree Fock; CAS=Complete Active Space; SCF = Self Consistent Field; MC = Multiple Configuration CI(F)S =Configuration Interaction (Full) Singles; SD = Single Determinant; FOMO = Floating Occupation Molecular Orbitals; SAC = Symmetry Adapted Cluster; PT= Perturbation Treatment; TD=Tamm- Dankoff approximation; B(3)LYP, PBE = different kinds of exchange and correlation density functionals.

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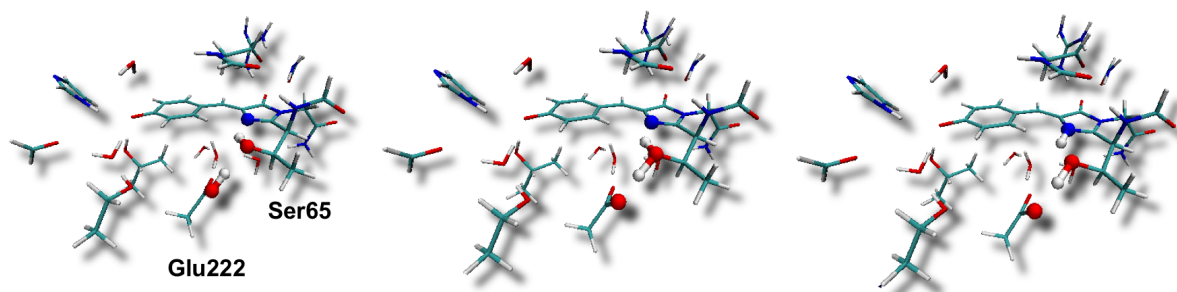s. Dong, J. et al. *J Am Chem Soc* **2006**, *128*, 12038

Figure 1: The formation of the zwitterionic state from the anionic by proton transfer from Glu222 via Ser65 in EGFP. Snapshots from a CP MD simulation on the excited state with the restricted open shell method.[1]
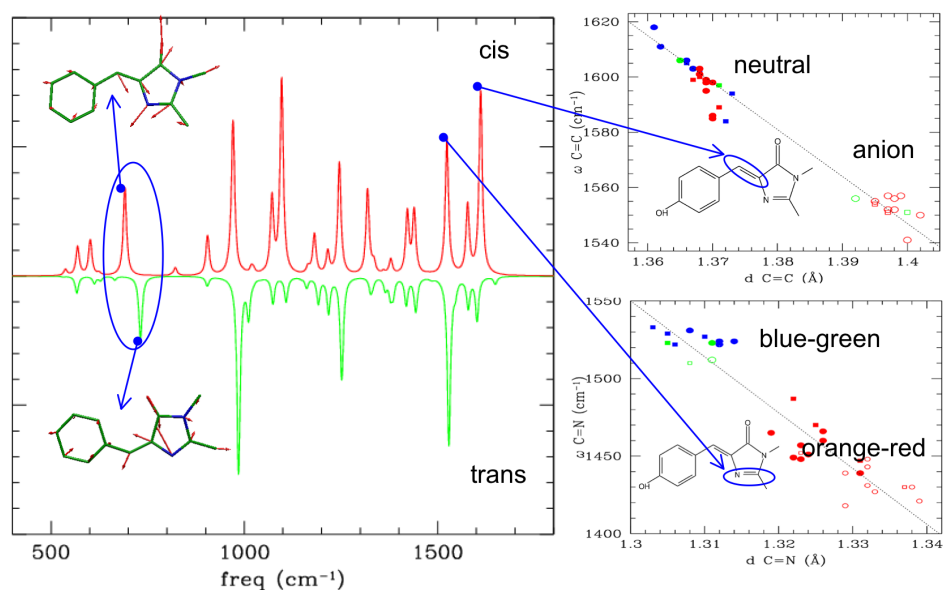

Figure 2: On-resonance Raman spectra of the cis (red) and trans (green) BFPF (obligate neutral) chromophore. The low frequency fingerprint band discriminating the two isomers is highlighted, as the two fingerprint modes corresponding to the C=C and C=N bonds vibrations. Their frequencies as a function of the bond length reported in the plots for all the chromophore types. The C=C band can discriminate the neutral from the anionic structures, the C=N band, the blue-green from the red-range ones (full symbols: neutral chromophores, empty, anionic chromophores; the color of the symbols roughly corresponds to the emitting color).[2]

References

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