Electronic structure aspects of photoconversions of the green fluorescent protein chromophore

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The unique properties of green fluorescent protein (GFP) exploited in novel bioimaging techniques have revolutionized many areas in life sciences, however, our mechanistic understanding of its function is still incomplete. I will present electronic structure calculations of the excited and ionized states of deprotonated 4'-hydroxybenzylidene-2,3-dimethylimidazolinone (HBDI anion). Our calculation offer a tentative structural explanation of the recently discovered oxidative redding of GFP. Relevant aspects of electronic structure methodology will also be discussed.

Literature:

1. E. Epifanovsky et. al., J. Chem. Theor. Comput. **5**, 1895 (2009)
2. Bogdanov et. al, Nature Chem. Biol. 5, 459 (2009)
3. E. Epifanovsky et. al., J. Chem. Phys., in press (2010)