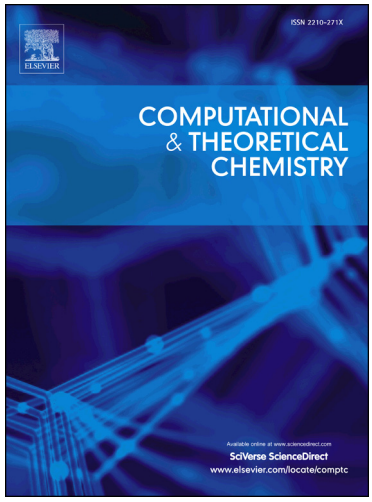

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Steering the excited state dynamics of a photoactive yellow protein chromophore analogue with external electric fields

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Abstract

The first excited state of the Photoactive Yellow Protein chromophore exhibits a strong charge transfer character and the dipole moments of the excited and ground state differ significantly. Furthermore, the excited state charge distribution changes during the isomerization of this chromophore. These observations suggest that external electric fields can be used to control photo-isomerization, providing a new concept for developing photochromic devices, such as e-paper or optical memory. To test this idea, we performed excited state dynamics simulations and static calculations of a PYP chromophore analogue (pCK^-) in an external electric field. By adjusting direction and strength of the field, we were able to control both selectivity (*i.e.,* which bond isomerizes) and efficiency (excited state lifetime) of the isomerization process. Simulations like these could potentially be useful in validating whether a given chromophore could be suitable for electrochromic applications.