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Theoretical Study of Chromophores for Biological Sensing: Understanding the Mechanism of Rhodol Based Multi-chromophoric Systems.

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Abstract. Development of two-photon fluorescent probes can aid in visualizing the cellular environment. Multi-chromophore systems display complex manifolds of electronic transitions, enabling their use for optical sensing applications. Time-Dependent Density Functional Theory (TDDFT) methods allow for accurate predictions of the optical properties. These properties are related to the electronic transitions in the molecules, which include two-photon absorption cross-sections. Here we use TDDFT to understand the mechanism of aza-crown based fluorescent probes for metals sensing applications. Our findings suggest changes in local excitation in the rhodol chromophore between unbound form and when bound to the metal analyte. These changes are caused by a charge transfer from the aza-crown group and pyrazol units toward the rhodol unit. Understanding this mechanism leads to an optimized design with higher two-photon absorption cross-sections to be used in medical applications.

Keywords: Time-Dependent Density Functional Theory; two-photon absorption cross-sections; optical sensors;