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Computational characterization of a visible light sensitized tellurorhodamine catalyst for thiol oxidation

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Homogeneous metal-catalyzed aerobic oxidation reactions have been of increasing interest due to the potential in green industrial applications. However, some industrially implemented methods require stoichiometric amounts of halogenated sacrificial electron acceptor to oxidize the Mn to M (n+2), the active oxidant species. Organo chalcogen dyes, and more specifically tellurium-containing dyes, have been demonstrated to photocatalytically oxidize thiol without the use of chemical oxidants. Computational modeling coupled to experimental results allows further understanding of oxidation and reduction mechanism associated with this catalytic cycle. This reaction is catalyzed by a visible-light-active, self-sensitized, tellurium-containing chromophore under ambient temperature and pressure. The tellurium-containing chromophore is a rhodamine-derivative that is photo-oxidized to the active telluroxide species without the addition of a photosensitizer or external oxidant (besides atmospheric oxygen). The mechanism of telluroxide formation and thiol to disulfide transformation were determined computationally and are supported by results from stop-flow spectroscopy experiments.

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