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# MOLECULAR LIGHT-TO-HEAT CONVERTERS: A NEW STRATEGY FOR AN OLD PROBLEM

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One major challenge in the twenty-first century is to increase global food production while the quality and quantity of arable land are diminishing. Central to this problem is the necessity to increase the yield of numerous important crop species and to find ways to extend geographical locations suitable for agriculture. One environmental constraint which hinders plant growth and development is cold stress. To protect plants from cold stress, we propose the use of molecular heaters, molecules which can absorb light at specific wavelengths and convert it into heat. Combining efforts from synthesis, spectroscopy, toxicology, and computational calculations, we present a series of suitable candidates to be used as molecular heaters.[1-3] Particularly, we use different quantum chemical approaches such as TDDFT, DFT/MRCI, CASSCF/CASPT2, and surface hopping simulations to elucidate the photodeactivation mechanism of these molecules. Our target chromophores are inspired by sinapoyl malate (SM), a naturally occurring molecule identified as an efficient photoprotective plant sunscreen.[4] Our SM derivatives present a fast and efficient relaxation mechanism that involves population transfer from an initially populated bright $^1\pi\pi^*$ state to a dark twisted charge transfer (TICT) state. This intermediate state is formed after a carbon-carbon double bond rotation and mediates an efficient internal conversion to the ground state through a conical intersection. The photoisomer formation is naturally prevented due to a symmetric substitution in one of the $sp^2$ carbons, ensuring almost complete recovery of the initial ground state. In summary, we present a class of nature-inspired molecules with an efficient nonradiative energy dissipation mechanism allowing the absorbed light to be converted into heat with minimal implication for photosynthesis. Considering their green synthesis, impressive photostability, and lack of critical toxicity, these molecules are promising molecular heaters for applications in agriculture, phototherapy, and generally where photothermal conversion is desirable.

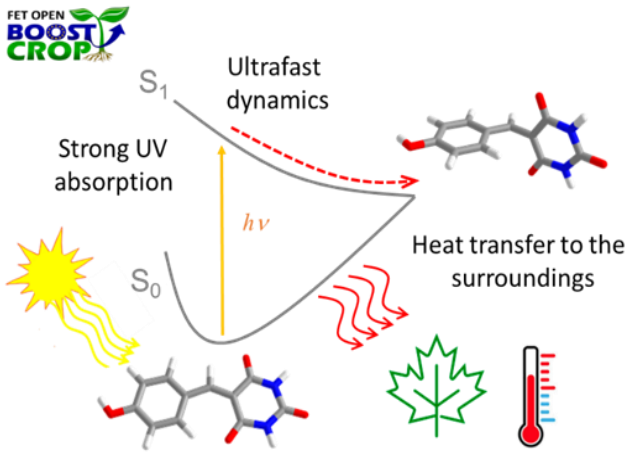


Figure 1. Schematic representation of the photophysics of molecular heaters.

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