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Photoisomerization dynamics of azobenzene materials for solar thermal fuels DAVID A. STRUBBE, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — A solar thermal fuel absorbs sunlight and stores the energy chemically via an induced structural change, which can later be reversed to release the energy as heat. Azobenzene molecules have a cis-trans photoisomerization with these properties, and hydrogen-bonding and packing via attachment to rigid template structures have shown promise in increasing the energy stored and the length of time it can be stored [A Kolpak et al, Nano Lett. 11, 3156-3162 (2011)]. Other important factors in determining the efficiency of a solar thermal fuel are the absorption cross-section and the quantum yield for photoisomerization, which must also be optimized for a successful material. We employ time-dependent density-functional theory (TDDFT) and the GW/Bethe-Salpeter formalism to calculate the optical absorption and dynamics in the excited-state to address these two factors. We use excited-state forces to map out potential-energy surfaces and follow the structural change after absorption for azobenzene-derived materials, to correlate the efficiency of photoisomerization with the functionalization and template.

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