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Hybrid chromophore/template nanostructures: a customizable platform material for emissions-free solar energy storage and conversion[1]

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By reversibly storing solar energy in the conformations of molecular photo-isomers, solar thermal fuels (STFs) provide a mechanism for emissions-free, renewable energy storage and conversion, all in a single system. Development of STFs as a large-scale clean energy technology, however, has been hampered by a number of technical challenges that beset many of the photo-isomers of interest. These challenges include low energy density, short storage lifetime, and low quantum yield of the photoisomerization reaction; a small overlap with the solar spectrum; and the irreversible degradation of the photo-active molecules upon repeated cycling. In this talk, I will discuss my work using first-principles computations to design new STFs that overcome these technical hurdles. I will present computational results on a range of novel STFs based on our recently proposed photo-isomer/template nanostructure concept [Kolpak and Grossman, Nano Letters 11, 3156 (2011)], illustrating that this approach enables enormous improvements with respect to the potential STFs studied in the past, leading to STFs with energy densities in the range of Li-ion batteries, storage lifetimes of up to a year, and increased quantum yield and absorption efficiency. I will also discuss preliminary experimental results on the synthesis and characterization of one of the predicted STFs based on azobenzene-derivitized carbon nanotubes. With a large range of the photo-isomer/template phase space yet to be explored, there are numerous exciting possibilites for further property enhancement and customization, suggesting that STFs could become a competitive renewable energy technology.

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