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Azonbenzene-functionalized carbon nanotubes as a high energy density solar thermal fuel ALEXIE KOLPAK, ENGIN DURGAN, JEFF GROSSMAN, Massachusetts Institute of Technology — Solar thermal fuels, which store energy from the sun in the chemical bonds of molecules, are a fascinating energy storage prospect: in principle they are 100% renewable, produce no emissions or by-products, are easily transportable in the form of liquids or powders, and can be recharged by the sun without any special equipment. However, adaptation of solar fuels as a viable, low-cost, large-scale means of energy storage will require the discovery of new materials other than the one known case based on Ruthenium that can perform the process over many cycles with no degradation. Here we discuss a novel approach to the design of solar fuels based on photoswitchable molecules covalently bonded to carbon nanotubes (CNTs). Using density functional theory, we examine the potential for maximizing the energy density via a combination of steric and intermolecular interactions between metastable azobenzene photoisomers and a CNT substrate. In addition, we investigate how a tuning parameter unique to the nanoparticle/molecule geometry — the packing density of the molecules on the nanotube — can be varied to produce significant, controlled changes in the transition pathway and barriers via ordered molecule-molecule interactions, potentially leading to new classes of nanoparticle-based solar fuels.

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