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Fundamental efficiency limit for solar thermal fuels DAVID A. STRUBBE, YUN LIU, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Solar thermal fuels (STFs) are an unconventional paradigm for solar energy conversion and storage which is attracting renewed attention: a material absorbs sunlight and stores the energy chemically via an induced structural change, which can later be reversed to release the energy as heat. An example is the azobenzene molecule which has a cis-trans photoisomerization with these properties, and can be tuned by chemical substitution and attachment to templates such as carbon nanotubes. By analogy to the Shockley-Queisser limit for photovoltaics (PV), we analyze the maximum attainable efficiency for STFs. The below-gap, above-gap, and recombination losses are similar to PV, but there are additional considerations about further losses, quantum yield, photostationary state, and interrelation with the storage lifetime, another key performance metric for STFs. We show constraints on feasible potential-energy surfaces for STFs, and compare to ab initio calculations and experimental measurements of the properties of STF materials.

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