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Design of novel solar thermal fuels with high-throughput ab initio simulations YUN LIU, JEFFREY GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — Solar thermal fuels (STF) store the energy of sunlight, which can then be released later in the form of heat, offering an emission-free and renewable solution for both solar energy conversion and storage. However, this approach is currently limited by the lack of low-cost materials with high energy density and high stability. Previously we have predicted a new class of functional materials that have the potential to address these challenges. Recently, we have developed an ab initio high-throughput computational approach to accelerate the design process and allow for searches over a broad class of materials. The high-throughput screening algorithm we have developed can run through large numbers of molecules composed of earth-abundant elements, and identifies possible metastable structures of a given material. Corresponding isomerization enthalpies associated with the metastable structures are then computed. Using this high-throughput simulation approach, we have discovered molecular structures with high isomerization enthalpies that have the potential to be new candidates for high-energy density STF. We have also discovered physical design principles to guide further STF materials design through the correlation between isomerization enthalpy and structural properties.

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