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Toward Molecular Solar-Thermal Energy Storage: Systematic Search for New Molecular Systems ENGIN DURGUN, VARADHARAJAN SRINIVASAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology, YOSUKE KANAI, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, GORDON WINTROP , JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, Massachusetts Institute of Technology — In the currently intensifying quest to harness solar energy for the powering of our planet, many efforts are centered around photo-induced generic charge separation, such as in photovoltaics, water splitting, and biologically inspired photosynthetic systems. An attractive alternative strategy would be to trap solar energy in the form of chemical bonds, ideally through the photo-conversion of a suitable molecule to a higher energy isomer, which, in turn, releases the stored energy by thermal reversal. Inspired by the discovery and investigations of fulvane-diruthenium, we explore strategies to discover new organometallic complexes that possess superior properties than organic molecules. We systematically search for complexes which are robust to storage cycles, easy to synthesize, tunable and which have high storage capacity and low UV excitation energies. Our analysis reveals that good organometallic candidates for solar-thermal energy storage systems can be identified and their performance can be improved through chemical substitution.

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