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Properties of Solar Thermal Fuels by Accurate Quantum Monte Carlo Calculations KAYAHAN SARITAS, CAN ATACA, JEFFREY C. GROSSMAN, Department of Materials Science and Engineering, MIT — Efficient utilization of the sun as a renewable and clean energy source is one of the major goals of this century due to increasing energy demand and environmental impact. Solar thermal fuels are materials that capture and store the sun's energy in the form of chemical bonds, which can then be released as heat on demand and charged again. Previous work on solar thermal fuels faced challenges related to the cyclability of the fuel over time, as well as the need for higher energy densities. Recently, it was shown that by templating photoswitches onto carbon nanostructures, both high energy density as well as high stability can be achieved. In this work, we explore alternative molecules to azobenzene in such a nano-templated system. We employ the highly accurate quantum Monte Carlo (QMC) method to predict the energy storage potential for each molecule. Our calculations show that in many cases the level of accuracy provided by density functional theory (DFT) is sufficient. However, in some cases, such as dihydroazulene, the drastic change in conjugation upon light absorption causes the DFT predictions to be inconsistent and incorrect. For this case, we compare our QMC results for the geometric structure, band gap and reaction enthalpy with different DFT functionals.

Kayahan Saritas
MIT

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