Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Addressing the challenges of solar thermal fuels via atomic-scale computational design and experiment ALEXIE KOLPAK, TIMOTHY KUCHARSKI, JEFFREY GROSSMAN, Massachusetts Institute of Technology — By reversibly storing solar energy in the conformations of photo-isomers, solar thermal fuels (STFs) provide a mechanism for emissions-free, renewable energy storage and conversion in a single system. Development of STFs as a large-scale energy technology has been hampered by technical challenges that beset the photo-isomers of interest: low energy density, storage lifetime, and quantum yield; UV absorption; and irreversible degradation upon repeated cycling. In this talk, we discuss our efforts to design new STFs that overcome these hurdles. We present computational results on various STFs based on our recently proposed photo-isomer/template STF concept [Kolpak and Grossman, Nano Letters 11, 3156 (2011)], as well as new experimental results on azobenzene-functionalized carbon nanotube STFs. Our approach yields significant improvements with respect to STFs studied in the past, with energy densities similar to Li-ion batteries, storage lifetimes $>$ 1 year, and increased quantum yield and absorption efficiency. Our strategy also suggests mechanisms for inhibiting photo-isomer degradation. With a large phase space yet to be explored, there remain numerous possibilites for property enhancement, suggesting that STFs could become a competitive renewable energy technology.

Alexie Kolpak
Massachusetts Institute of Technology

Date submitted: 07 Nov 2011 Electronic form version 1.4