

Atomic-scale design of materials for solar energy storage and conversion

A.M. Kolpak and J.C. Grossman

Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, USA
e-mail: kolpak@mit.edu

One of the most fascinating possibilities of materials research involves using fundamental knowledge of atomic-scale behavior to systematically design materials with novel mechanical, chemical, and electronic properties. In this talk, I will illustrate some of these possibilities with two examples from our recent work using first-principles density functional theory (DFT) to develop new materials for solar energy harvesting and conversion.

EXAMPLE I: PHOTOVOLTAICS

Exciton recombination plays a significant role in decreasing the efficiency of photovoltaic devices. In the first part of this talk, I will discuss a new materials concept, explored via DFT, that exploits the atomic-scale properties of semiconductor heterointerfaces to simultaneously drive electron-hole separation and eliminate recombination at defects. Using GaAs as an example, I will show that the introduction of atomic-layer defects with nanoscale periodicity can be used to create (a) large electric fields throughout the active material and (b) alternating quasi-two-dimensional electron and hole conducting layers/carrier channels. These properties lead to a material in which electron-hole pairs are separated by strong electric fields over nanoscale distances, as illustrated in Fig. 3. In addition, defects aggregate to the metallic interfaces, at which they are compensated. By driving exciton separation and removing recombination centers, such superlattices could potentially enable “dirty” materials to work as efficiently as their high-purity counterparts.

EXAMPLE II: SOLAR THERMAL FUELS

Solar thermal fuels (STFs), which reversibly store solar energy in the conformations of molecular photoisomers, as illustrated schematically in Fig. 1,

have exciting potential as emissions-free, renewable energy storage and conversion systems. Despite the evident advantages of STFs, however, their development as a large-scale clean energy technology has been hampered by a number of key technical challenges that beset many of the photoisomers of interest. These challenges include low energy density, short storage lifetime, small overlap with the solar spectrum, and irreversible degradation upon repeated cycling. In the second part of this talk, I will describe our computational efforts to overcome these technical hurdles. I will show that, using our recently proposed photoisomer/template platform to tune chemical interactions between bound photoisomers, we obtain a range of novel STFs (Fig. 2) with predicted energy densities comparable to Li-ion batteries, year-long storage capabilities, and enhanced optical properties. I will also present preliminary experimental results on predicted STFs composed of azobenzene-derivatized carbon nanotubes. With a large range of the photoisomer/template phase space yet to be explored, there are numerous exciting possibilities for further property enhancement and customization, suggesting that STFs could provide a practical means of storing solar energy.

CONCLUSIONS

These examples provide a glimpse of the exciting possibilities inherent in an atomic-scale approach to engineering materials properties, and furthermore, suggest that such materials could play an important role in mitigating our current energy challenges.

REFERENCES

- [1] A.M. Kolpak and J.C. Grossman, *Azobenzene-Functionalized Carbon Nanotubes As High-Energy Density Solar Thermal Fuels*, *Nano Letters* **11**, 3156 (2011).

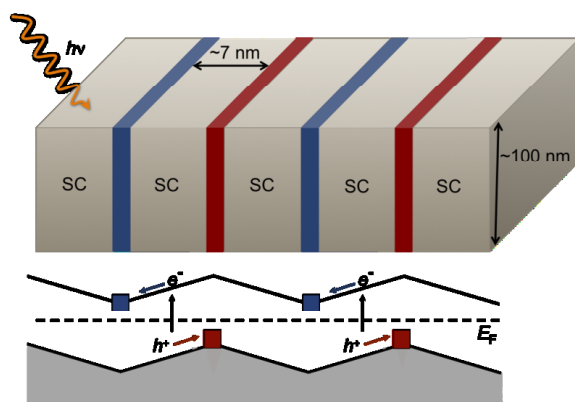


Fig. 1. Schematic of the proposed nanoscale superlattice (top) and the resulting band structure (bottom). Blue and red regions indicate the quasi-2D electron and hole conducting gases that result from the introduction of atomic-layers of Se and Zn, respectively.

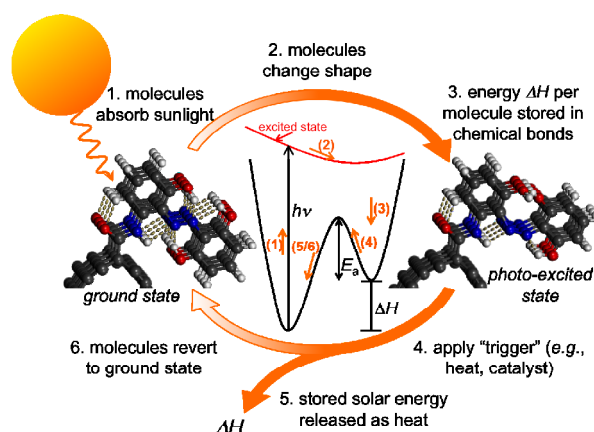


Fig. 2. Schematic illustrating the operation of a solar thermal fuel.

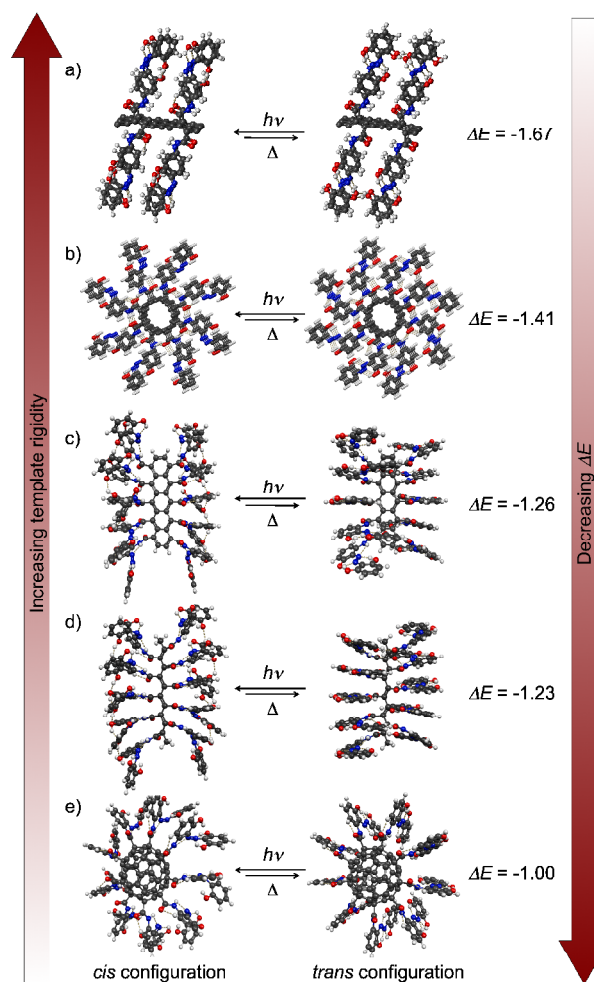


Fig. 3. Atomic structure and energy stored per molecule for azobenzene derivatives on various template materials. For comparison, the energy stored per molecule in gas phase azobenzene is -0.59 eV. White, grey, blue, and red spheres represent H, C, N, and O atoms, respectively.