Simulations on the atomic scale of materials for solar energy

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My background

Studied chemistry and physics in college (Univ of Chicago)

Studied physics and nanoscale science and engineering for PhD (at UC Berkeley)

Postdoc in materials science and engineering

Here: involved with chemistry and materials science graduate groups

Bringing together different disciplines is key for solar research!

My first involvement with solar: undergraduate summer research project...
Photovoltage with PbS Nanocrystal Films

Long-term goal: photoelectrochemical (PEC) cell to compete with silicon solid-state solar cells.

Reported success with PbS quantum dots as sensitizer for TiO$_2$.

Can it be done with just PbS?
Approaches for solar research

Tracks: materials, devices, optics, manufacturing, deployment, economics and society

Goals: lower cost, higher efficiency, better reliability, new functionality (storage, building integration, weight, flexibility)

Improvement of existing technologies

Or development of new materials and paradigms
Why computation?

*Experimental challenges:*

Time scale to absorb light: femtosecond, $10^{-12}$ s

Size scale for motions of atoms: Ångström, $10^{-10}$ m

But natural time and spatial scales for calculations!

Calculations can be faster, cheaper, and more versatile than experiments.

Goal: design and understand materials to be later made, studied, and used

**Quantum mechanics: for electrons**

Schrödinger equation

$$H \Psi = E \Psi$$

Hard to solve for many electrons in material – need a computer
Computational resources

Laptop, 8 cores

MERCED cluster, SE2 basement, ~2000 cores

Edison (100k) and Cori (600k) supercomputers,
National Energy Research Supercomputing Center,
Lawrence Berkeley National Laboratory,
Berkeley, CA
Pentacene: an organic semiconductor

Cheap, flexible

New opportunity: singlet fission!

How atoms move after absorbing light
Utilization of solar energy: intermittency problem

1) What do we do at night and when it’s cloudy?

2) How do we level demand for our current grid and backup generation?

- Solar hot water
- Batteries
- Pump water uphill
- Solar water splitting
- Molten salts
Solar thermal fuels: integrated reversible storage

sunlight $\rightarrow$ chemical energy $\rightarrow$ heat

$trans$: lower energy

$cis$: higher energy

trans-azobenzene: calculated forces and experiment

Thermodynamic efficiency limit for photovoltaics

below gap: not absorbed

above gap: thermalized to $E_g$

radiative recombination


“Shockley-Queisser limit”

32% at $E_g = 1.2$ eV for unconcentrated, single-junction solar cell
Thermodynamic efficiency limit for photovoltaics

Understand deficiencies and room for improvement

Motivate new paradigms:
- multi-junction cells
- spectrum-splitting
- carrier multiplication
- hot-electron devices
- intermediate-band cells
- up- or down-conversion
- ...


Our analysis: solar thermal fuels has the same thermodynamic limit as photovoltaics!
Degradation and reliability

Best Research-Cell Efficiencies

- **Multijunction Cells (2-terminal, monolithic)**
  - LM = lattice matched
  - IM = metamorphic
  - IM = inverted, metamorphic
  - Three-junction (concentrator)
  - Three-junction (non-concentrator)
  - Two-junction (concentrator)
  - Two-junction (non-concentrator)
  - Four-junction or more (concentrator)
  - Four-junction or more (non-concentrator)

- **Single-Junction GaAs**
  - Single crystal
  - Concentrator
  - Thin-film crystal

- **Crystalline Si Cells**
  - Single crystal (concentrator)
  - Single crystal (non-concentrator)
  - Multicrystalline
  - Silicon heterostructures (HIT)
  - Thin-film crystal

- **Thin-Film Technologies**
  - CIGS (concentrator)
  - CIGS
  - CdTe
  - Amorphous Si:H (stabilized)

- **Emerging PV**
  - Dye-sensitized cells
  - Perovskite cells (not stabilized)
  - Organic cells (various types)
  - Organic tandem cells
  - Inorganic cells (CZTSSe)
  - Quantum dot cells (various types)

- **a-Si/c-Si tandem HIT 28%**
- **Perovskites (not stabilized) 22%**
- **a-Si:H (stabilized) 14%**

https://www.nrel.gov/pv/assets/images/efficiency-chart.png
Amorphous silicon

crystalline: short- and long-range order (periodic)

amorphous: only short-range order

Combined together: heterojunction with intrinsic thin layer (HIT cell)
Light-induced degradation in amorphous silicon

PhD student, Enrique Guerrero

How does light absorption change or damage the structure?

Staebler-Wronski effect

Maybe related to moving Si-H bonds at voids
Light-induced degradation in hybrid perovskites

PhD student, Kuntal Talit

$(\text{CH}_3\text{NH}_3)\text{PbI}_3$

What kind of damage is happening?
How can we design a more stable material or device?

Phonon eigenvector

Wanyi Nie et al., Nat. Commun. 7, 11574 (2016)
Undergraduate work in my research group

Two computer science majors

Computational nanoscience toolkit online

Speeding up C++ code for making amorphous structure

3D printing for materials visualization
How can undergraduates get involved?

Talk to faculty whose work you find interesting!

Apply for a Research Experience for Undergraduates (REU) program: at one of dozens of university sites around the country, get paid by the National Science Foundation to do a research project for the summer.

Apply for the Science Undergraduate Laboratory Internships (SULI) at one of the Department of Energy National Laboratories: get paid to do research at Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Sandia National Laboratory (Livermore), etc. Mostly summer but fall/spring possible too.

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Opportunities:
**Summer undergraduate research fellowship, due Feb 28**  
MACES undergraduate fellowship (apply in fall)  
Summer internships at NASA research centers (apply in fall)

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