Silicon solar cells: illuminating barriers from the nano-scale to the "scientist-scale"

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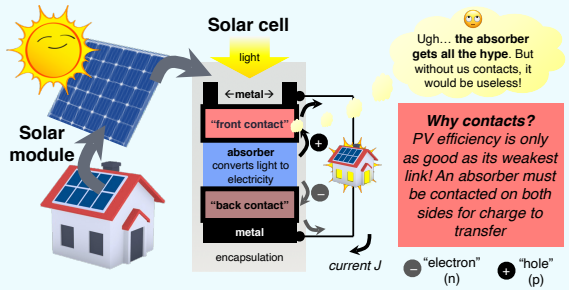
Silicon solar cells efficiencies are limited by bad contacts. Can we use inverse design to find a better "hole-selective contact"?

Back to basics

How do solar photovoltaics (PV) work?

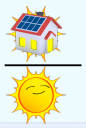


Ugh… **the absorber gets all the hype**. But without us contacts, it would be useless!

Why contacts? *PV efficiency is only as good as its weakest link! An absorber must be contacted on both sides for charge to transfer*

PV efficiency

$\eta = \frac{\text{Energy out}}{\text{Energy in}}$



Silicon heterojunction (SHJ)

η =	
Theory	32.7%
Cell	26.7%
Module	~20%
10 years	~17%

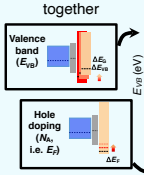
10% of market share by 2024

But discrepancy with theoretical efficiency! Why?

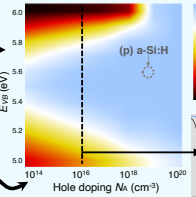
Simulating materials properties

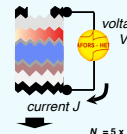
Multi-parameter analysis is key

VB and doping must be optimized together

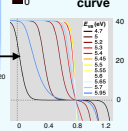


Simulated performance





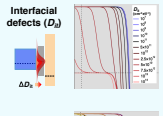
Current-voltage (*J-V*) curve



Band bending

Performance drops can be explained by recombination and loss of quasi-fermi level splitting

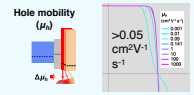
Defects and thickness matter

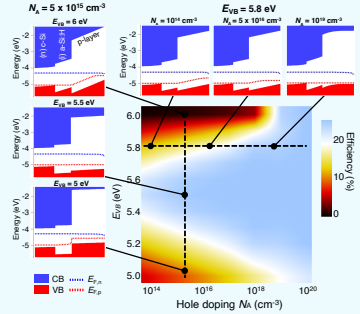


If the p-layer is doped high enough the valence band alignment does NOT have to be as sharp!

If VB is sufficiently aligned, doping does not have to be very high

Mobility less important

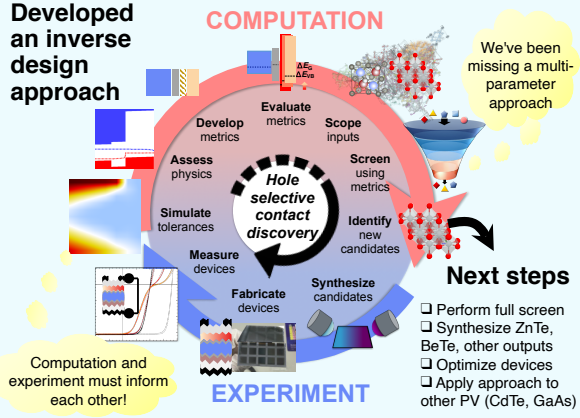




These design parameters and their tolerances can now be used as inputs for inverse design searches

Conclusions

Developed an inverse design approach



We've been missing a multi-parameter approach

Computation and experiment must inform each other!

Next steps

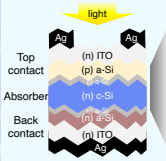
- ❑ Perform full screen
- ❑ Synthesize ZnTe, BeTe, other outputs
- ❑ Optimize devices
- ❑ Apply approach to other PV (CdTe, GaAs)

References

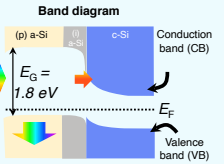
[1] NREL, (2020). "Best Research-Cell Efficiency Chart."
[2] **Woods-Robinson, R.**, et al. (2020). *Journal of photovoltaics*
[3] **Woods-Robinson, R.**, et al. (2021). *2020 47th IEEE Photovoltaic Specialists Conference (PVSC)*
[4] **Woods-Robinson, R.**, et al. (2020). *Chemical Reviews*, 120(9), 4007-4055.

Nanoscale barriers

SHJ schematic



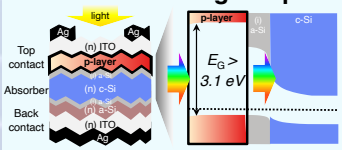
Challenges in SHJ



Parasitic absorption: The top contact is not transparent enough! Band gap E_G is too small

Can we find a transparent hole selective contact, aka "p-layer", to replace (p) a-Si?

New SHJ device



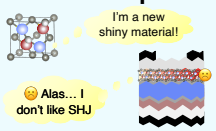
Design requirements

- ❑ p-type material (how much?)
- ❑ More transparent than a-Si
- ❑ VB "aligned" with c-Si's VB; no contact resistance
- ❑ Low interface recombination

But these are qualitative…

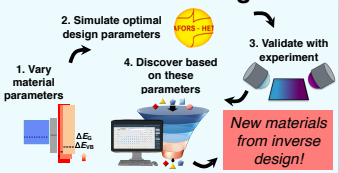
Theory-experiment barriers

Status quo



Predictions haven't worked… are we designing wrong?

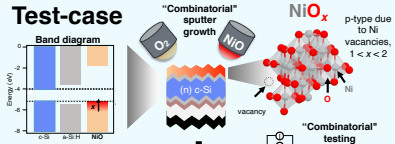
"Inverse design"



New materials from inverse design!

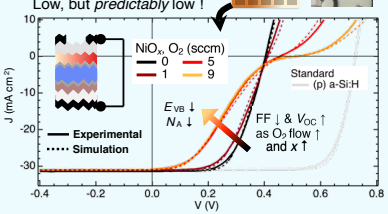
Experimental validation

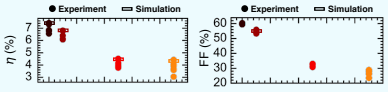
Test-case

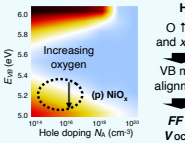


PV efficiency

Low, but *predictably* low !







Hypothesis:

O ↑ and x ↑ → VB mis-alignment → FF ↓ V_{OC} ↑

SiO_2 at interface → D_{it} ↑ → FF ↓ V_{OC} ↓

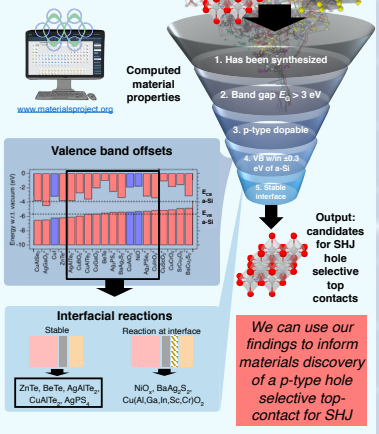
Experimental trends corroborate VB position and materials properties in our simulations

Design new materials

Updated design requirements

- ❑ Band gap E_G > 3 eV (as expected)
- ❑ E_{VB} aligned to 5.5 eV: w/in ±0.3 eV for $N_A > 10^{18}$ cm^{-3}, or w/in ±0.1 eV for $N_A > 10^{16}$ cm^{-3} for $D_{it} < 10^{11}$
- ❑ Higher D_{it}: sharper E_{VB} and N_A requirements
- ❑ Mobility > 0.05 cm^{2}V^{-1}s^{-1} (less restrictive!)

Inverse design screening "funnel"



We can use our findings to inform materials discovery of a p-type hole selective top-contact for SHJ

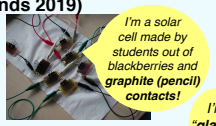
Scientist-society barriers

How can we connect with our communities to build trust and communicate these challenges?

Cycle for Science, founded by Rachel Woods-Robinson (Berkeley) and Elizabeth Case (Columbia), takes scientists on bicycle trips around the world to stop in classrooms and teach hands-on lessons about renewable energy and climate change

Scientists: what we do → Science background → Interactive activity → Climate discussion

DIY solar cells (Netherlands 2019)



DIY glaciers (NY 2019)

"Sol cycle" (cross-USA 2015, CA 2017)

Are you a scientist interested in joining a future trip? We'd love to have you! Reach out at ***wecycleforscience@gmail.com***

Contact about contacts: rwoodsrobinson@lbl.gov

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