# Theory, Modeling, Simulation & Understanding PV Devices

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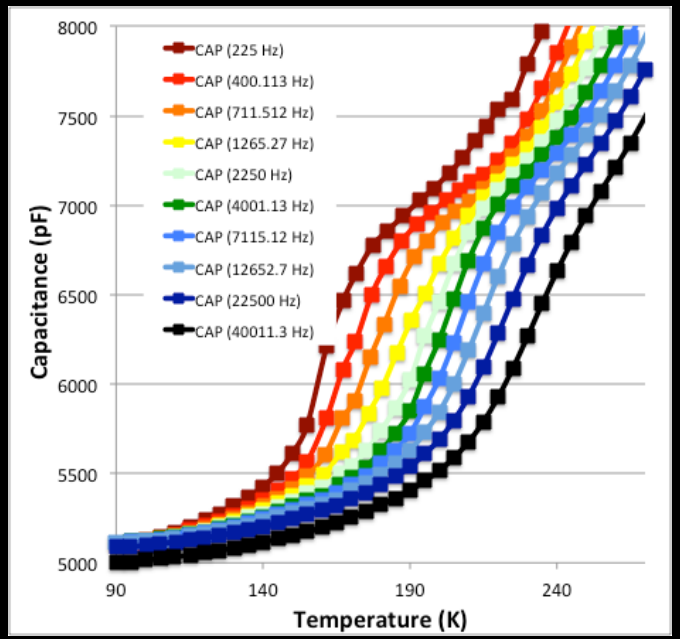
# What does my data mean?

- Experiments are usually the fastest way to try things.
- Experiments lie (but so do models) – how to tell?
- Interpreting results correctly and using them to drive next experiments is hard.
- Theory: general case explanation, not application specific.
- Modeling: specific application of theory to a given case but not applied to specific data.
- Simulation: using models to replicate specific data and project to untried cases.

# What does my data mean?

- Consider common experimental results such as C/V admittance spectroscopy. Simple models & explanations only take you so far.




CIGS Device in the dark:

Admittance step: carrier escape from a defect. Simple theory gives the defect state depth well.

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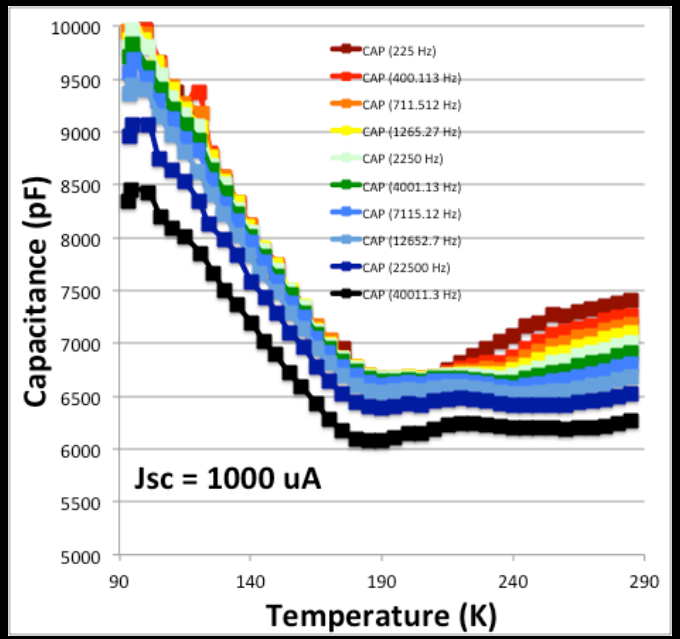


CIGS Device in the light:

This is very hard to understand. Need a detailed device model to understand.

# Multiscale Modeling Steps

- Validate data – did my experiment lie? Quick & dirty "back of the envelope" works.
- Extract critical effects from known problems with known solutions.
- Analyze critical problems in detail to understand their underlying causes.
- Connect critical problems to specific defects by atomistic approaches.
- Test possible approaches to solving the critical problem.

# Multiscale Modeling

Jsc > 50 mA/cm2?

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Shunt resistance removed?

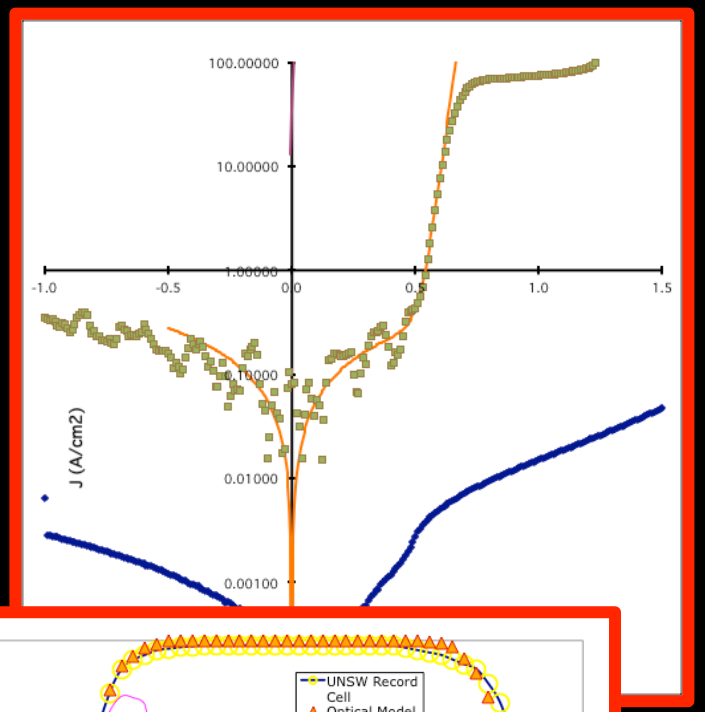
Inversion of the heterojunction?

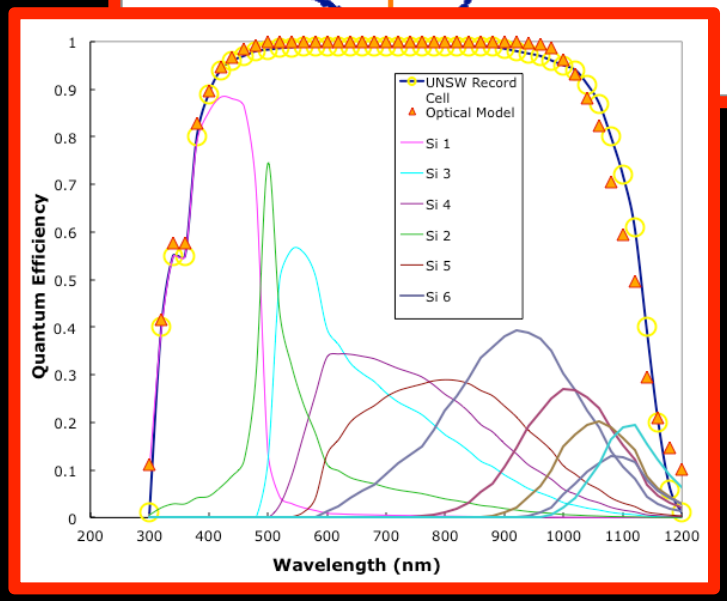
Can Cd dope CIGS at the junction?

What if CdS is replaced with ZnS?

# Options to Understanding

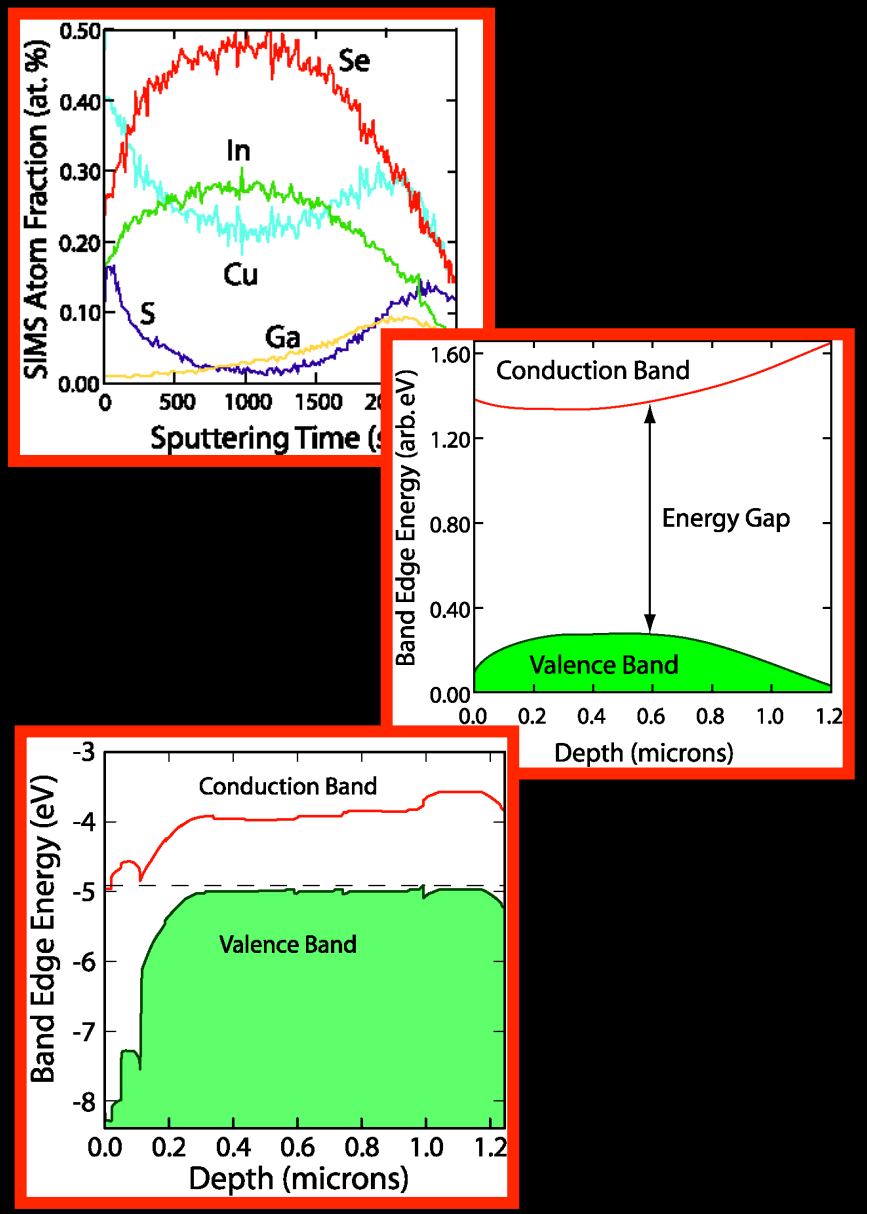
- Spreadsheets/fast fits: can yield a very fast interpretation of data.
- Little underlying physics.
- Helps to extract known but solvable components of behavior.
- Helps select the next scale of model to apply.



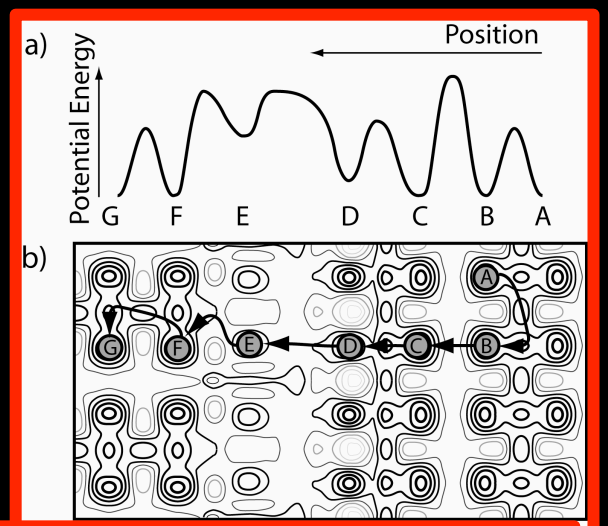
# Options to Understanding

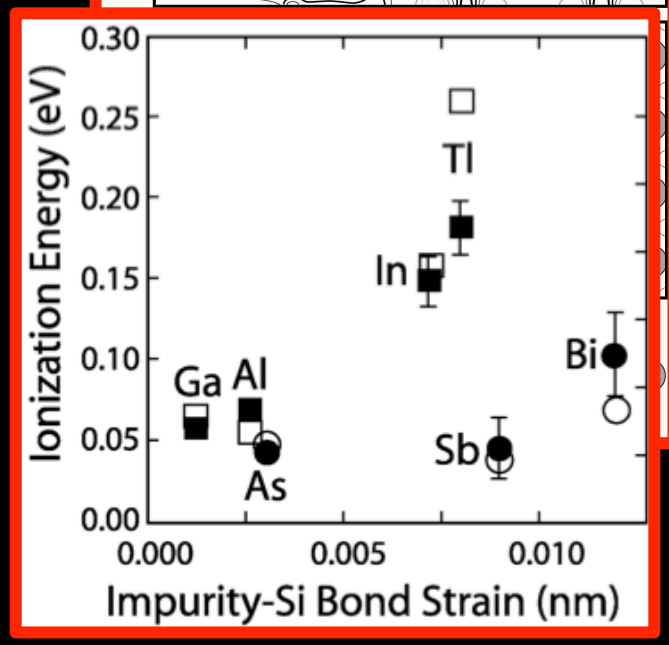
- Detailed device model to quantitatively relate specific observation to specific defect or property.
- Need enough experimental data to separate sufficient from necessary explanations.



# Options to Understanding

- DFT: good if the effects you care about are on a scale of 64-256 atoms or so.
- Simulation cell size gets to be a limitation rapidly.
- As with TEM, it is easy to miss key issues due to small scale.
- You can learn a lot just from the Harrison atomic orbital energies.



# Summary:

- All levels of simulation and modeling are critical to rapid prototyping and process development.
- Quick & dirty analysis is fastest for prototyping
- Device models are critical to diagnosing details of limitation to devices.
- Ab-initio techniques are important to testing hypothesized atomic-scale defects