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.
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 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

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

Jsc > 50 mA/cm²?
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