Unified Numerical Solver for Modeling Device Metastabilities in CdTe Thin-Film PV

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**Project Objective:** The Unified Solver proposed to be developed as part of this project will enable the analysis of polycrystalline PV devices at unprecedented depth. Greater depth, however, implies a greater challenge in obtaining accurate values in the Solver inputs. In this project, input parameters will be taken from the literature or derived from first-principle calculation, and will be fine-tuned through validation experiments. Systematic approaches to calculate the key input parameters will be developed. While the uncertainty in the input parameters may present the most significant risk to this project, a working Solver will allow us to validate results and chemical trends in a targeted approach. The existence of GBs cannot be ignored and will be embraced as a critical feature in the Solver. Additionally, a device solver will be an integral component of the Unified Solver, since drift and diffusion processes are influenced by the presence of electric fields, which may well be influenced by GBs and other impurities. A closed solution to the entire system will be developed.

**Need for PREDICTS**

Without “unified infrastructure” discrepancies do not exist at critical levels.

**Device Characterization**

- Needs accurate models to be interpreted correctly
- Models and calibrates parameters but need parameters and Fermi level

**Physical Model**

- Defects interaction energy
- Defect system
- Grain boundary geometry
- Defect / carrier kinetics
- Device stack (opt.)

**Mathematical Model**

- Implicit Reaction Scheme isolated from Diffusion-Reaction Equations
- Avoid negative concentration
- Maintain conservation

- Solution of Diffusion-Diffusion Equations
- Solute-Gamma model for GBs and other impurities

**Experimental Data**

**Single Crystal CdTe Anneal**

- ZnTe-Cu vs CdTe
- Cu Drop
- Diffusion Depths
- Smooth Diffusion Tail

**1D Simulations**

- Cu & CdCl₂ defect system investigated first:
  - Saturation behavior established as equilibrium of defect chemistry.
  - Smooth diffusion tail formed by internal electric field
  - Cu drop near interface achieved by Cu back diffusion during cool down.

- Compensation between Cu₂Cd and Cu₂Cl₂ 3 x 10⁻¹⁰ cm⁻² hole density

**Discrepancy presented between DFT and fitted diffusion parameters.**

- The employed diffusion barrier (0.72eV) was found to be close to the DFT calculated dissociation energy of Cu₂Cl₂ (0.71eV)

- Expand our model with formation and dissociation of Cu complexes

**DFT Calculations**

**Goal:** Develop defect diffusion theory. Calculate the defect properties such as:

- defect formation energy
- ionization energy
- defects interaction energy
- diffusion path
- diffusion energy barrier, etc.

in both bulk and grain boundaries.

**Dissemination on nanoHUB.org**

1D solver: 53 Users + 1 Citation
2D solver: 45 Users

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