Structural and Chemical Features Contributing to Defect Tolerance of Binary Semiconductors

Or, how can we make really cheap solar cell materials?

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Hybrid perovskites are surprising!

1) Astounding efficiency gains

**Best Research-Cell Efficiencies**

- **Multijunction Cells** (2-terminal, monolithic)
  - LM = lattice-matched
  - IM = inverted, metamorphic
- **Three-junction (concentrator)**
- **Two-junction (concentrator)**
- **Two-junction (non-concentrator)**
- **Four-junction (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**
- CIS (concentrator)
- CIGS
- C4In
- 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)

Chart from NREL National Center for Photovoltaics, accessed 2018

~18 years

~26 years

~37 years

~4.5 yrs

~27 years

~26 years

~27 years

~37 years
Hybrid perovskites are surprising!

1) Astounding efficiency gains
2) Unconventional fabrication techniques

Typical high-performance semiconductor manufacturing

- High temperature!
- High vacuum!
- High purity!

Hybrid perovskites manufacturing:

- Ambient temperature and pressure, precursors and processing done in a normal glovebox in a regular lab!

So how are they so good?!?*

* Other than the toxicity and lack of stability...
Defect Tolerance!

50% relative efficiency loss at over 100 TIMES the concentration of iron!
Why are shallow defects good?

\[ U_{SRH} \propto e^{E_t - E_i} \]

“deep” defect state = BAD

“shallow” defect state = LESS BAD

DFT Defect Calculations

\[ \Delta H_{D,q}(E_F) \approx \left[ E_{D,q} - E_{\text{host}} \right] + qE_F + \sum_{\alpha} n_{\alpha} \mu_{\alpha} + E_{\text{corr}} \]

- Electrochemical potential \((electrons)\)
- Chemical potential \((for\ atoms\ added/removed)\)
  (here \(1 \times \mu_B\))

Compensate for supercell size effects


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Defect Energy Diagrams

\[ \Delta H_{D,q}(E_F) \approx [E_{D,q} - E_{\text{host}}] + qE_F + \sum_\alpha n_\alpha \mu_\alpha + E_{\text{corr}} \]

\[ \Delta H \]

\[ -2 \quad 0 \quad +1 \quad +2 \]

VBM

\[ E_F \]

VBM + Eg
How does defect tolerance happen?

In $^{+1, +3}$

Sn $^{+2, +4}$

Sb $^{+3, +5, -3, -2}$

Tl $^{+1, +3}$

Pb $^{+2, +4}$

Bi $^{+3, +5, -3, -2}$
But they don’t have shallow defects!

~30 separate DFT calculations on $\mathcal{O}(100)$ atoms.
Updating our understanding

change the **structure**  
change the **energies** (chemistry)
Back to those binary iodides

(a) InI

(b) TlI

(c) SnI₂

(d) PbI₂

(e) SbI₃

(f) BiI₃

Testing the new theory

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Updated Theory of Defect Tolerance: Cation vacancies (chemistry)

a. deep cation vacancy

Updated Theory of Defect Tolerance: Anion vacancies (structure)