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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BLUE WATERS

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NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Photovoltaics Research Laboratory

Hybrid perovskites are surprising!

1) Astounding efficiency gains

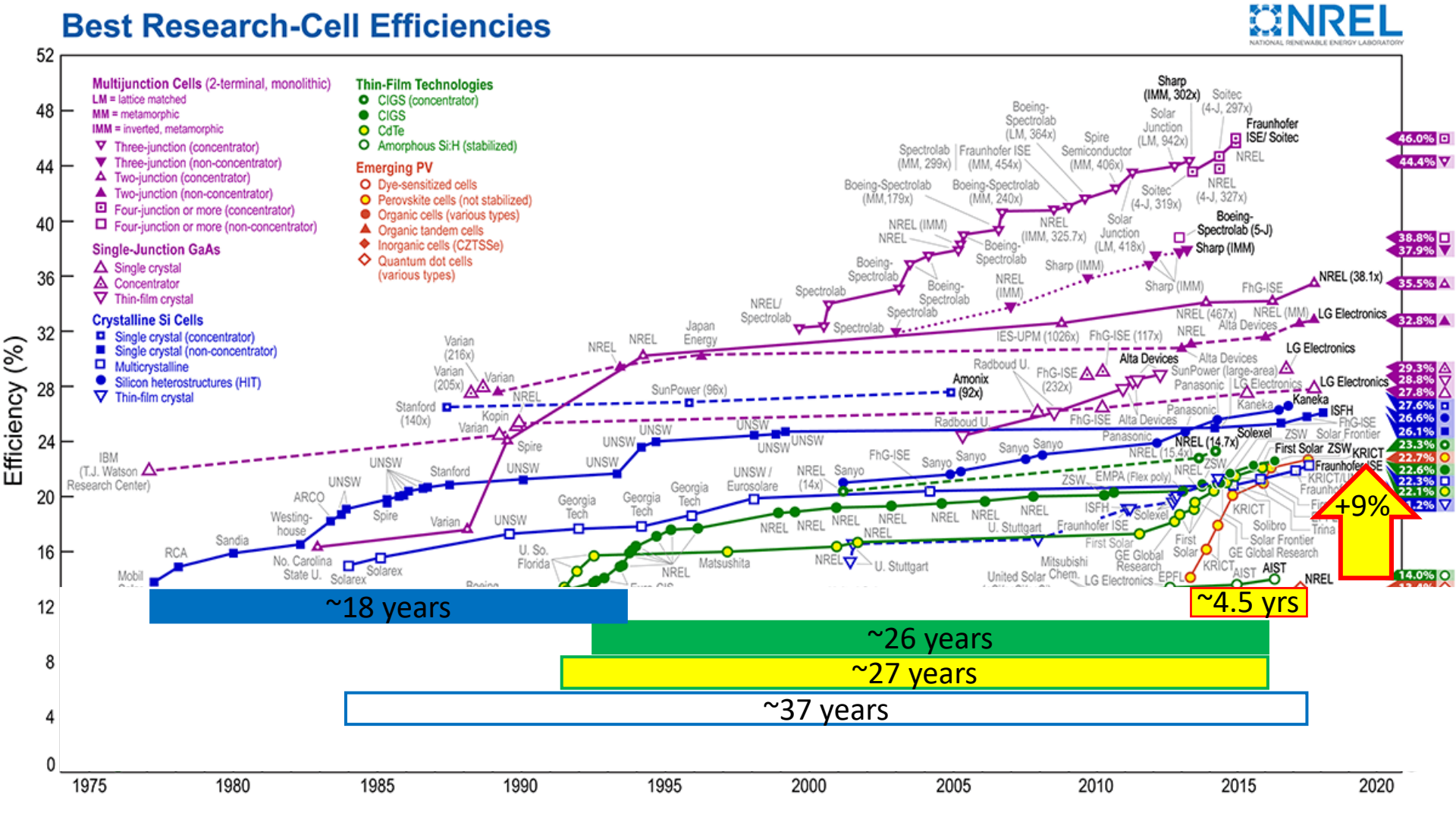
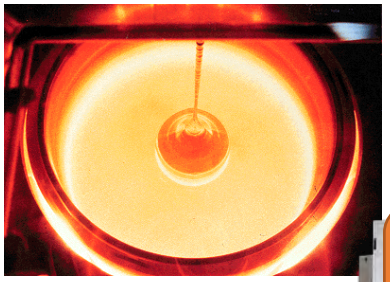


Chart from NREL National Center for Photovoltaics, accessed 2018

Hybrid perovskites are surprising!

1) Astounding efficiency gains
2) Unconventional fabrication techniques

Typical high-performance semiconductor manufacturing



High temperature!

High vacuum!

High purity!

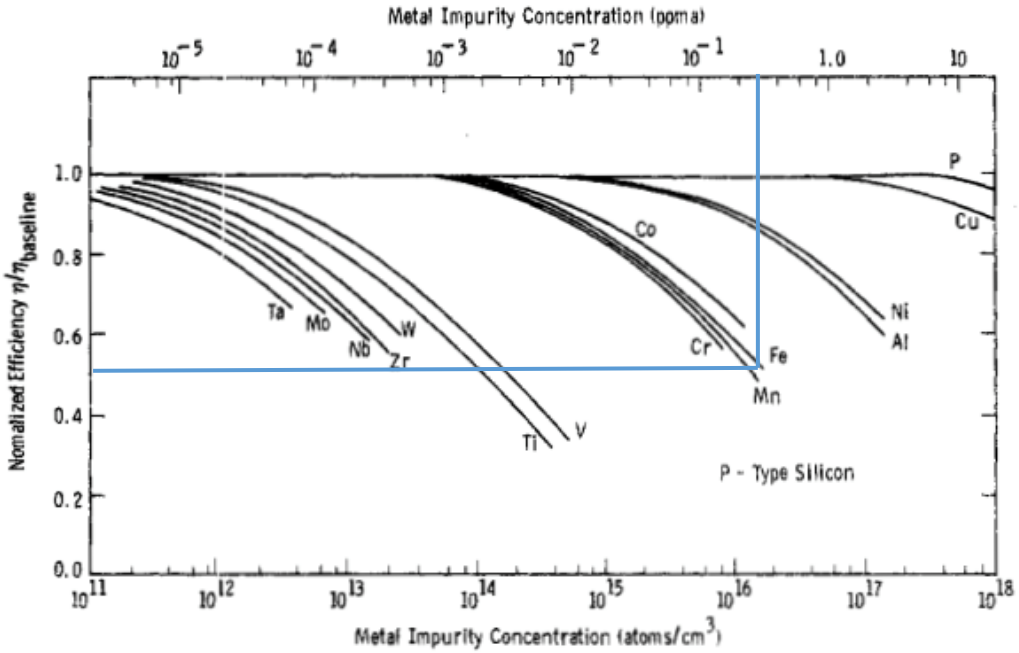
Hybrid perovskites manufacturing:

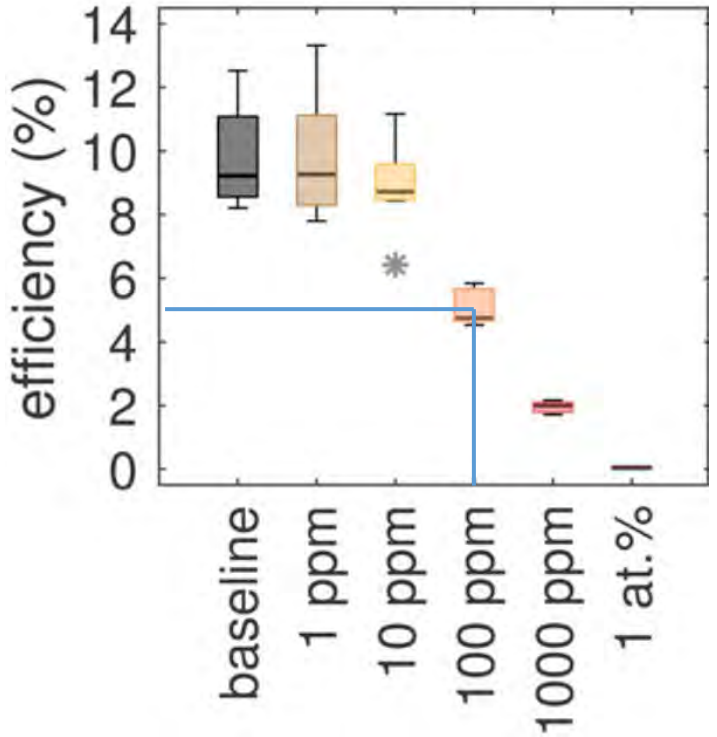
Ambient temperature and pressure, precursors and processing done in a normal glovebox in a regular lab!

So how are they so good?!?*

* Other than the toxicity and lack of stability…

Defect Tolerance!

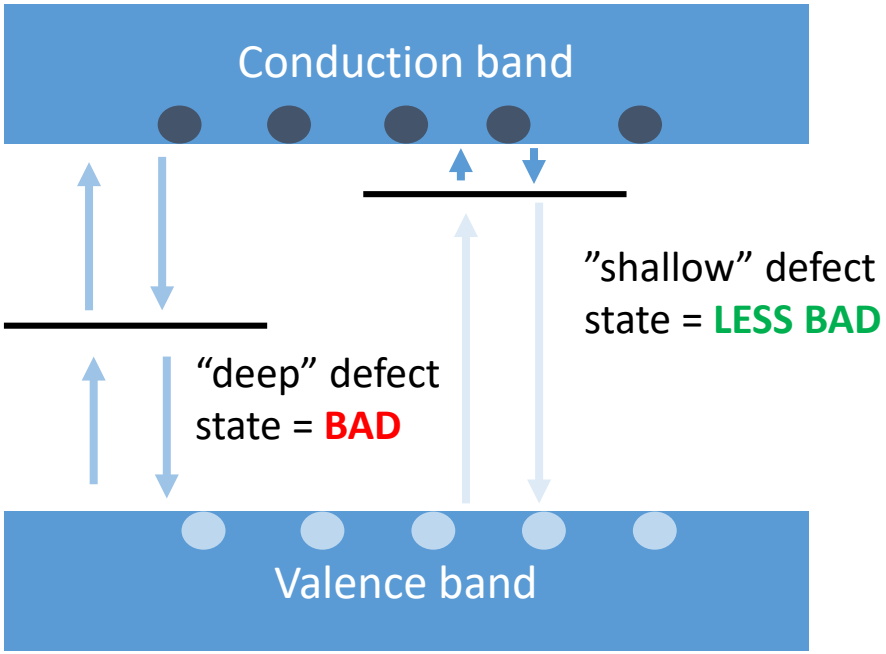




50% relative efficiency loss at over 100 TIMES the concentration of iron!

J. R. Davis *et al.*, "Impurities in silicon solar cells," in *IEEE Transactions on Electron Devices*, vol. 27, no. 4, pp. 677-687, April 1980.
Poindexter, J. R., *et al. (*2017). High Tolerance to Iron Contamination in Lead Halide Perovskite Solar Cells. *ACS Nano*.

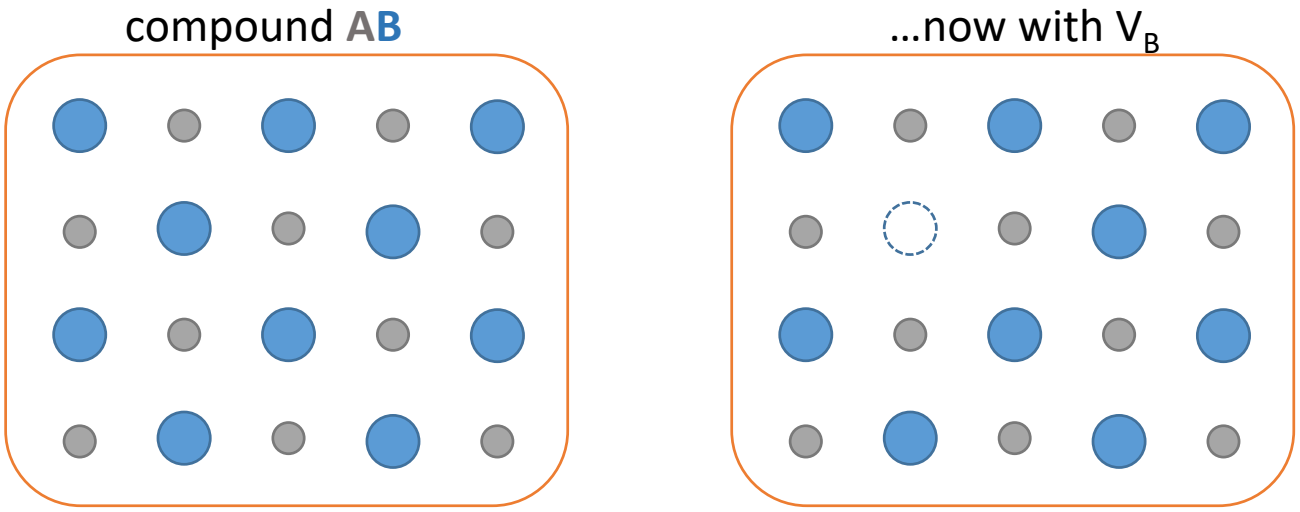
Why are shallow defects good?



$$U_{\mathrm{SRH}} \propto e^{|E_t - E_i|}$$

Shockley, W. and Read, W. T. (1952) ‘Statistics of the Recombination of Holes and Electrons’, *Physical Review*, 87(46), pp. 835–842.
Hall, R. N. (1952) ‘Electron-Hole Recombination in Germanium’, *Physical Review*, 87(2), p. 387.

DFT Defect Calculations



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

Electrochemical potential *(electrons)*

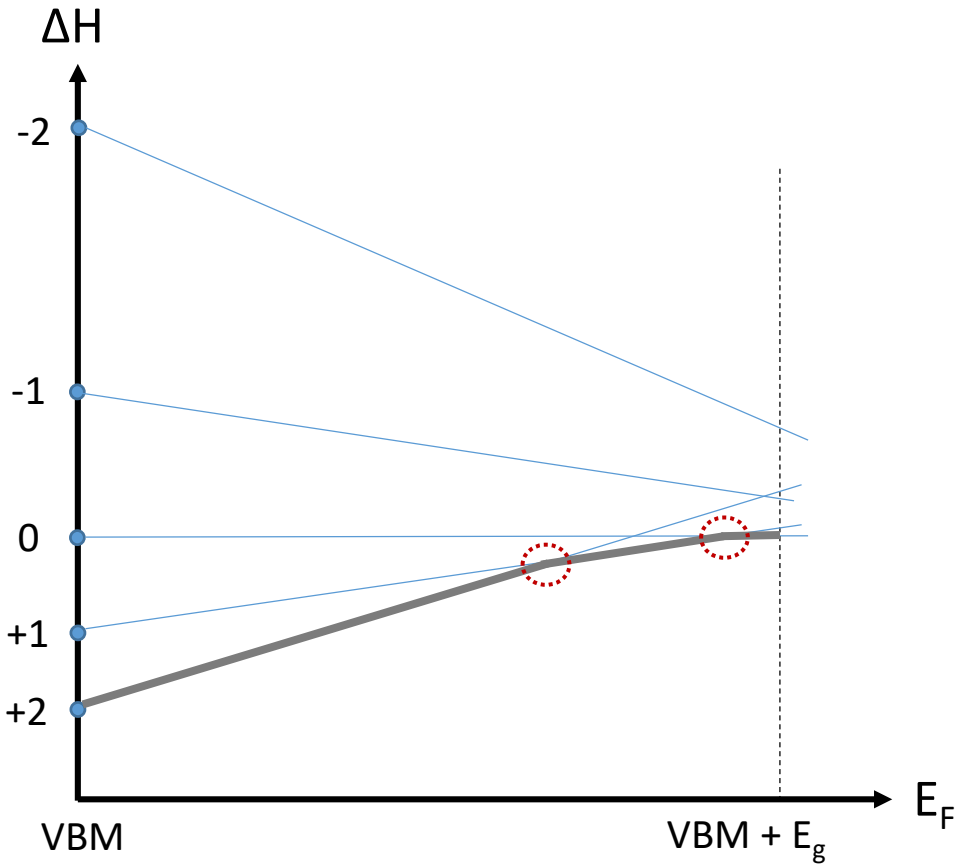
Chemical potential *(for atoms added/removed)* (here 1 x μ_B)

Compensate for supercell size effects

Lany, S. and Zunger, A. (2008) 'Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs', *Physical Review B - Condensed Matter and Materials Physics*, 78(235104), pp. 1–25.

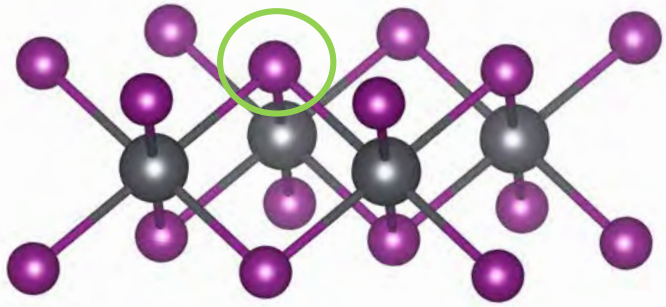
Defect Energy Diagrams

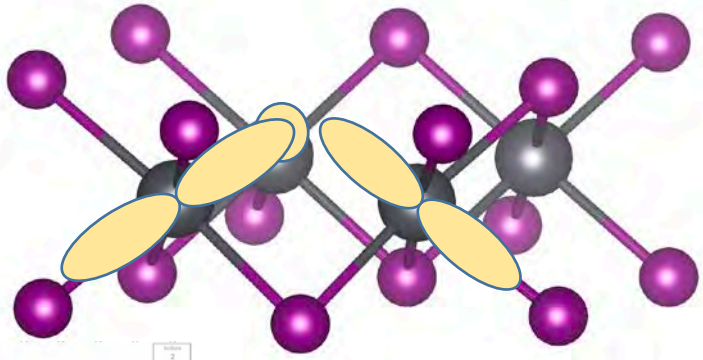
$$\Delta H_{\mathrm{D,q}}(E_F) \approx [E_{\mathrm{D,q}} - E_{\mathrm{host}}] + qE_F + \sum_{\alpha} n_\alpha \mu_\alpha + E_{\mathrm{corr}}$$

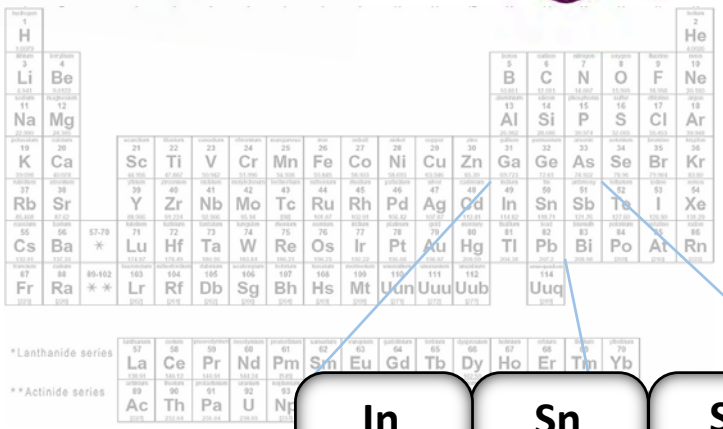


Lany, S. and Zunger, A. (2008) 'Assessment of correction methods for the band-gap problem and for finite-size effects in supercell defect calculations: Case studies for ZnO and GaAs', *Physical Review B - Condensed Matter and Materials Physics*, 78(235104), pp. 1–25.

How does defect tolerance happen?



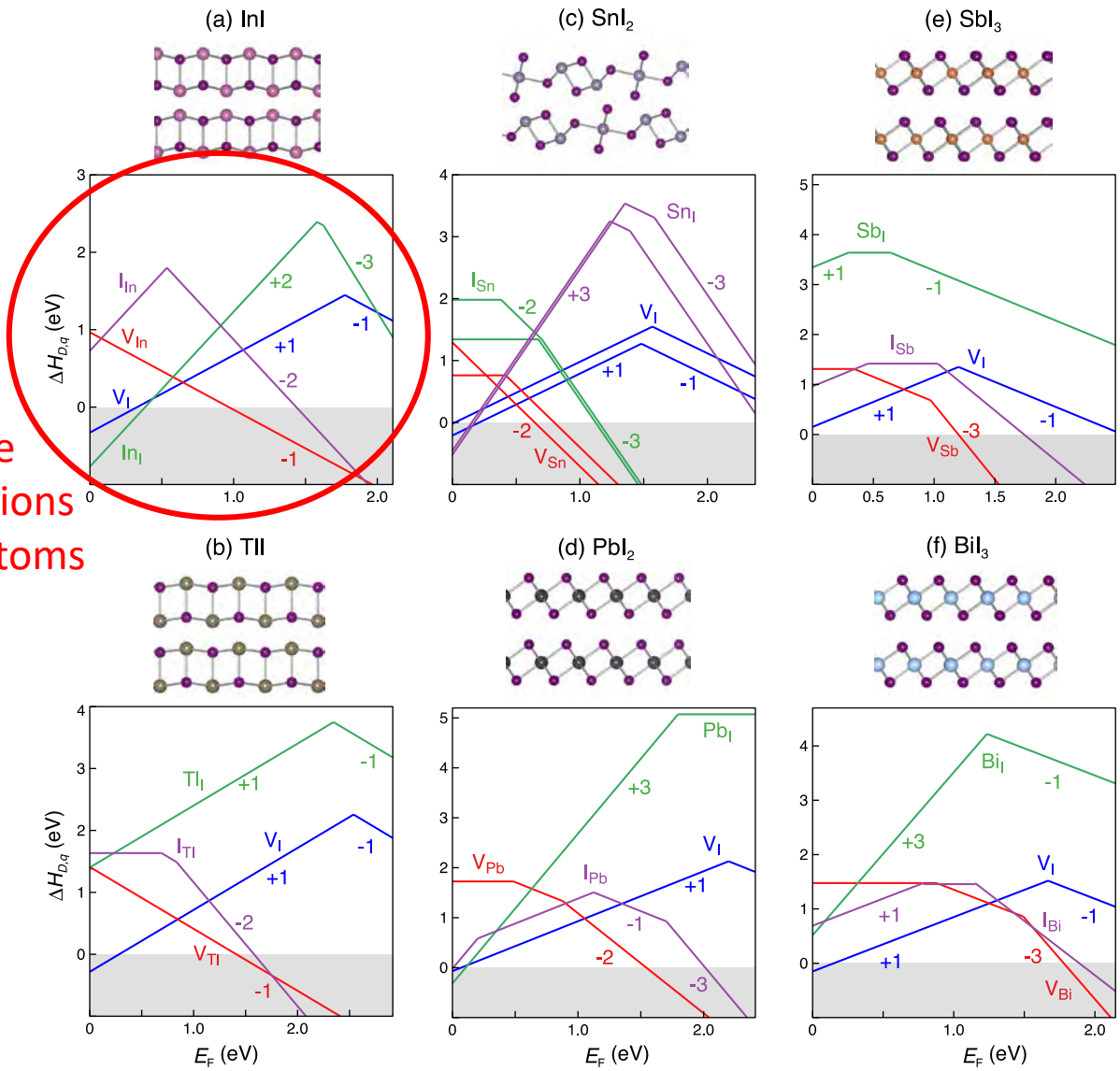




In +1,+3	**Sn** +2,+4	**Sb** +3,+5, -3,-2
Tl +1,+3	**Pb** +2,+4	**Bi** +3,+5, -3,-2

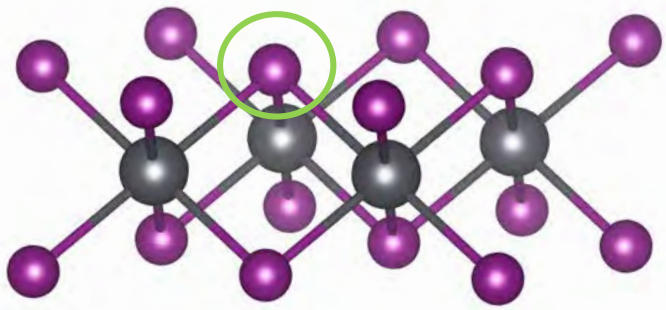
But they don't have shallow defects!

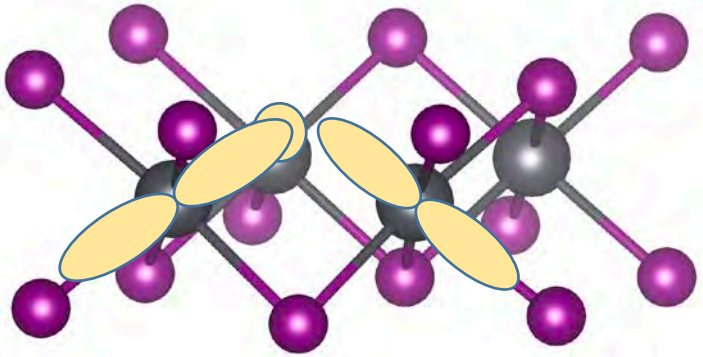
~30 separate DFT calculations on $\mathcal{O}(100)$ atoms

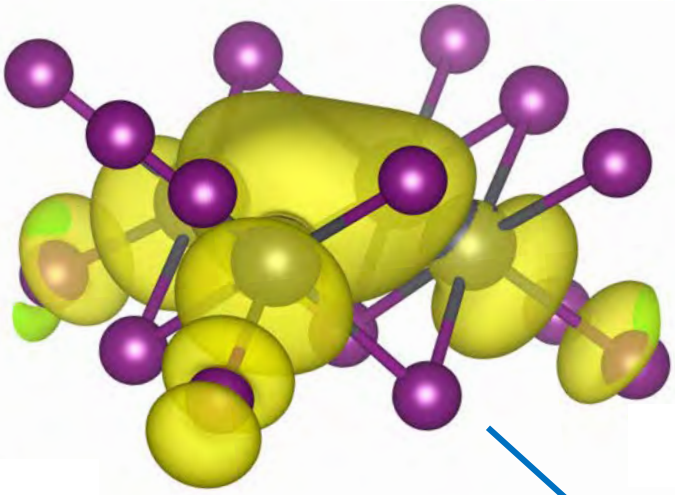


Kurchin, R. C., Gorai, P., Buonassisi, T., & Stevanović, V. (2018). Structural and Chemical Features Giving Rise to Defect Tolerance of Binary Semiconductors. *Chemistry of Materials*, under revision.

Updating our understanding



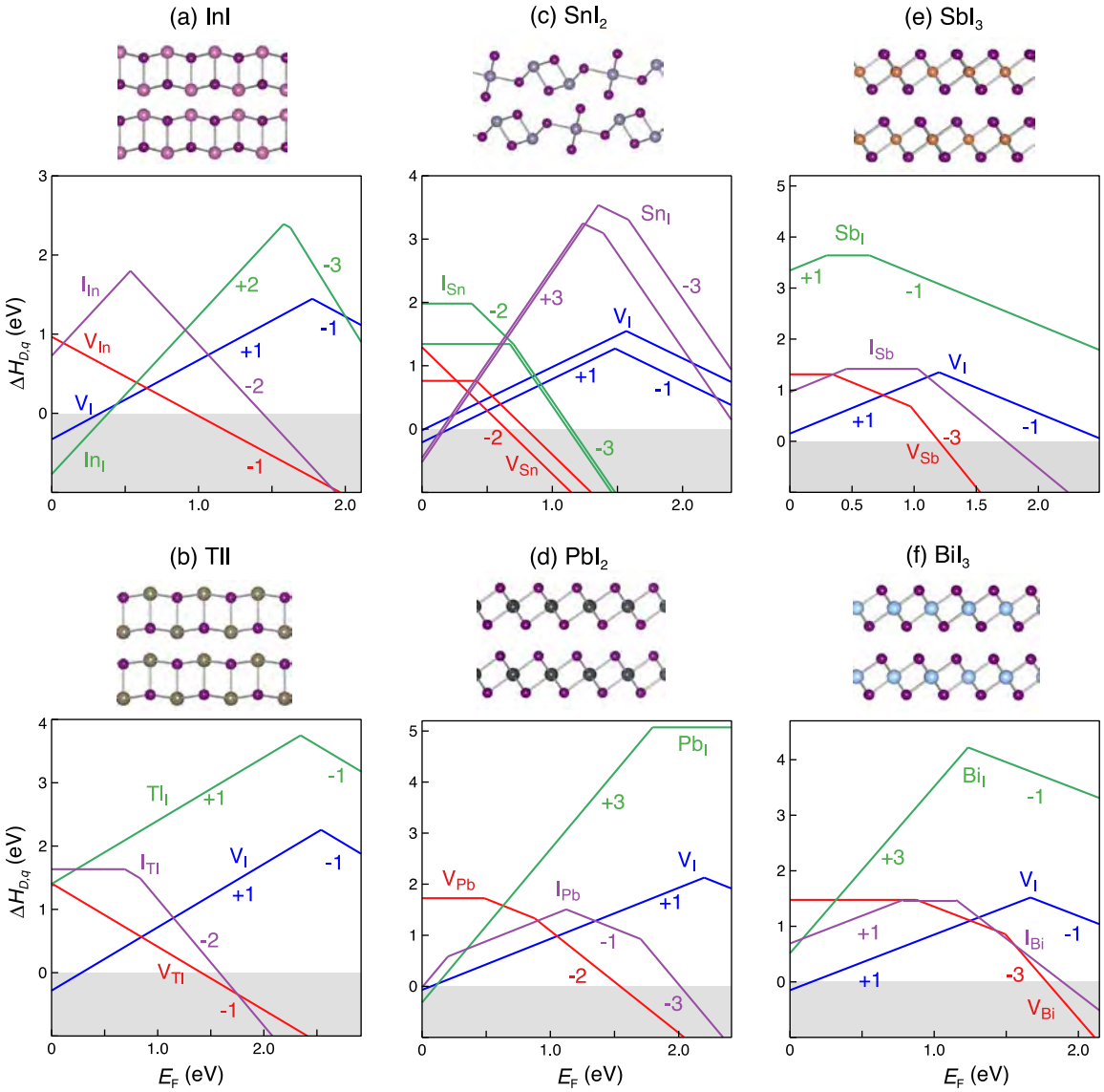




change the **structure**

change the **energies** (chemistry)

Back to those binary iodides



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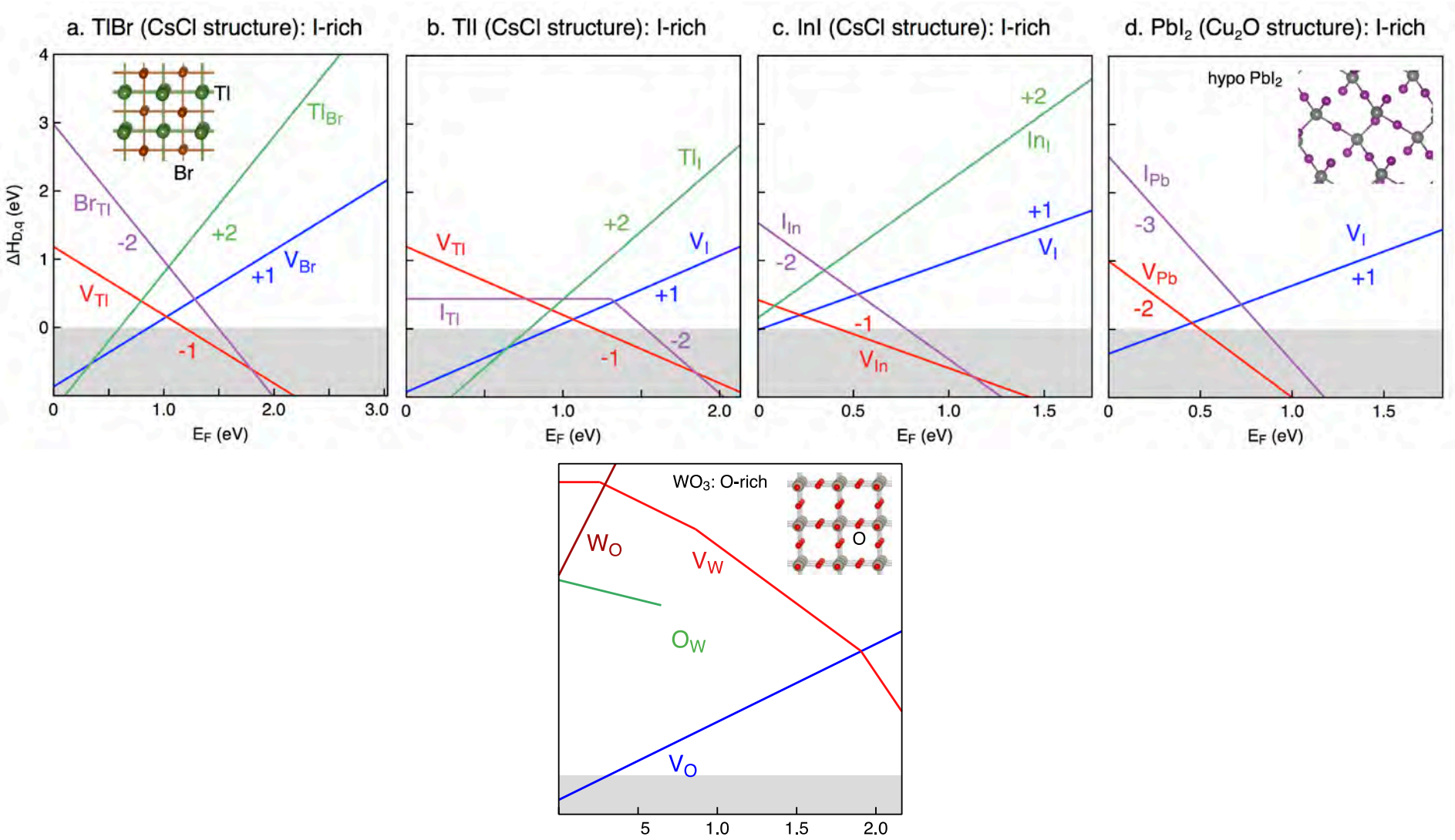
Testing the new theory



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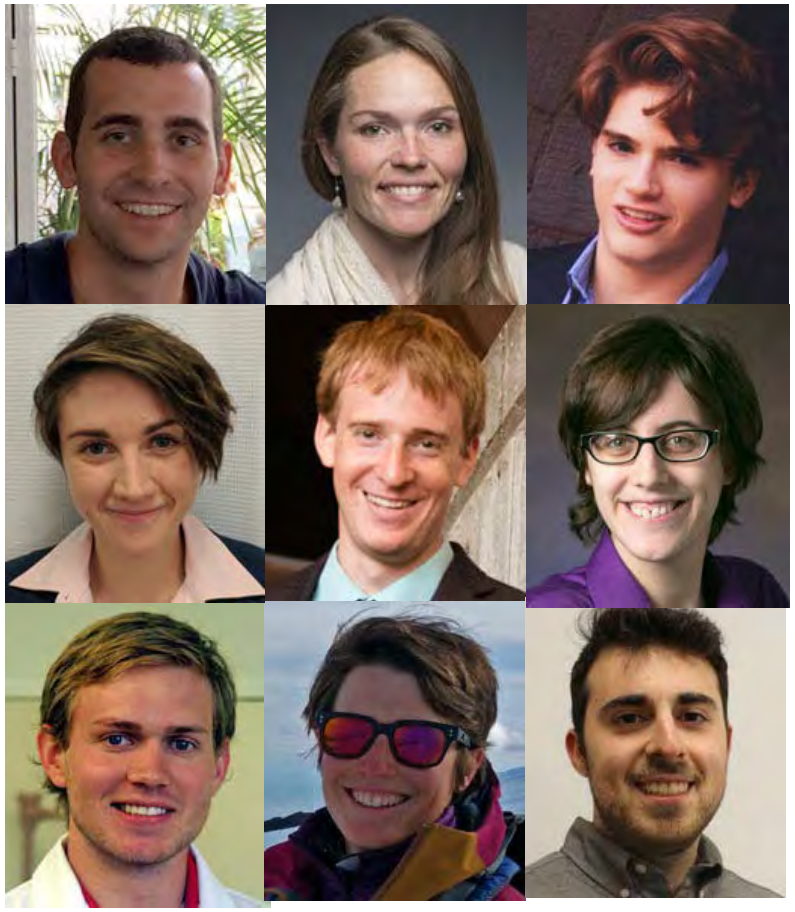
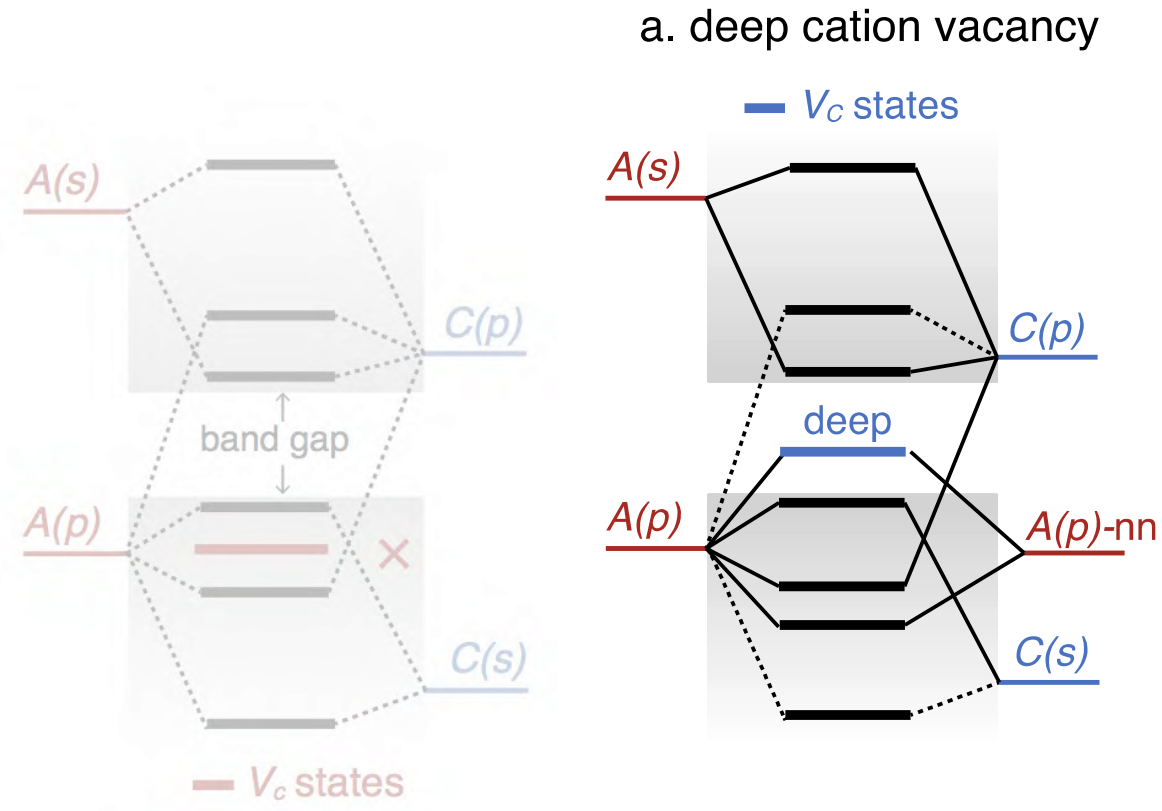
Thanks, Blue Waters!

- BW Graduate Fellowship gave me intellectual independence and confidence in my research
- And a great community!



Updated Theory of Defect Tolerance: Cation vacancies (chemistry)



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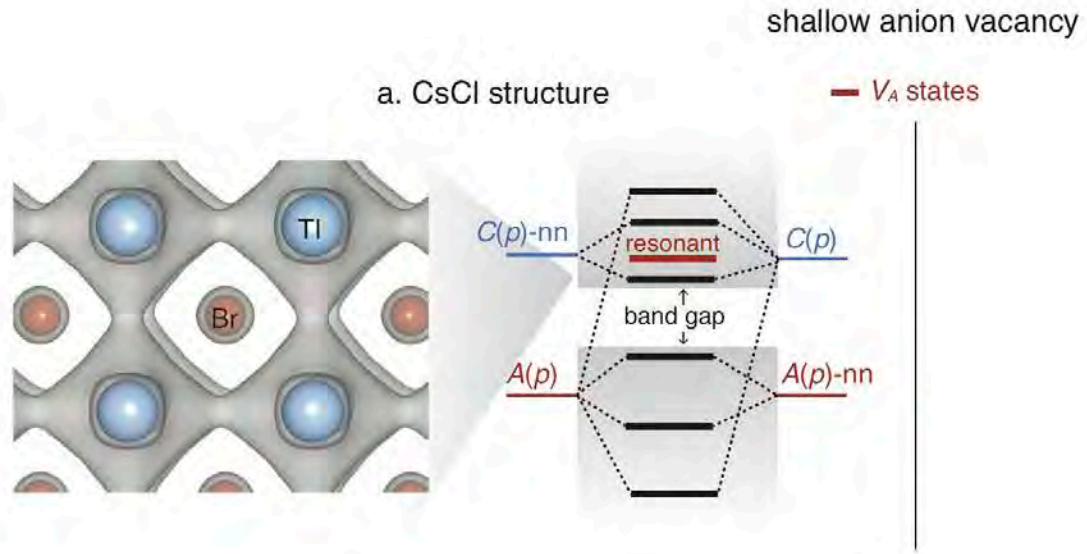
Updated Theory of Defect Tolerance: Anion vacancies (structure)



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