
Developing a Data Format and Repository for Sharing First-principles Defect Calculations



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What can we learn from defect calculations?

- We can learn about the defect chemistry, which is important in applications such as: thermoelectric, photovoltaic, etc.
- First-principles defect calculations are now mature, are routinely done and provides useful insights

npj | Computational Materials

ARTICLE OPEN

First-principles calculation of intrinsic defect chemistry and self-doping in PbTe

Anuj Goyal^{1,2}, Prashun Gorai^{1,2}, Eric S. Toberer^{1,2} and Vladan Stevanović^{1,2}

cm CHEMISTRY OF MATERIALS

Article
pubs.acs.org/cm

Thermoelectric Performance and Defect Chemistry in n-Type Zintl KGaSb₄

Brenden R. Ortiz,^{*,†} Prashun Gorai,[‡] Vladan Stevanović,^{§,§} and Eric S. Toberer^{*,†,‡}

cm CHEMISTRY OF MATERIALS

Article
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Searching for "Defect-Tolerant" Photovoltaic Materials: Combined Theoretical and Experimental Screening

Riley E. Brandt,^{*,†} Jeremy R. Poindexter,[‡] Prashun Gorai,^{§,§} Rachel C. Kurchin,[†] Robert L. Z. Hoye,^{†,¶} Lea Nienhaus,[‡] Mark W. B. Wilson,^{†,¶} J. Alexander Polizzotti,[†] Raimundas Sereika,^{||} Raimundas Žaltauskas,^{||} Lana C. Lee,[†] Judith L. MacManus-Driscoll,[⊥] Mounqi Bawendi,[†] Vladan Stevanović,^{§,§} and Tonio Buonassisi[†]

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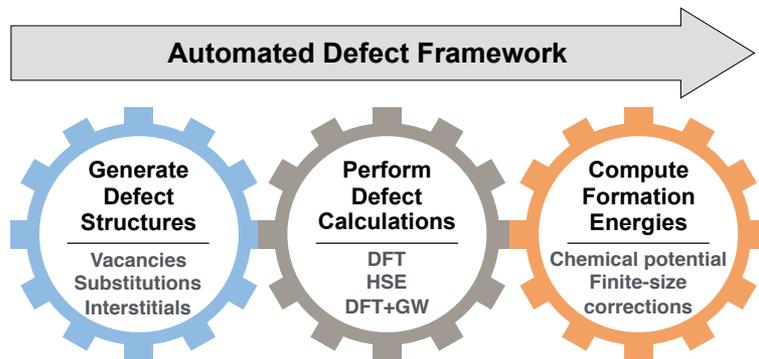
COMPUTATIONAL MATERIALS SCIENCE

Editor's Choice

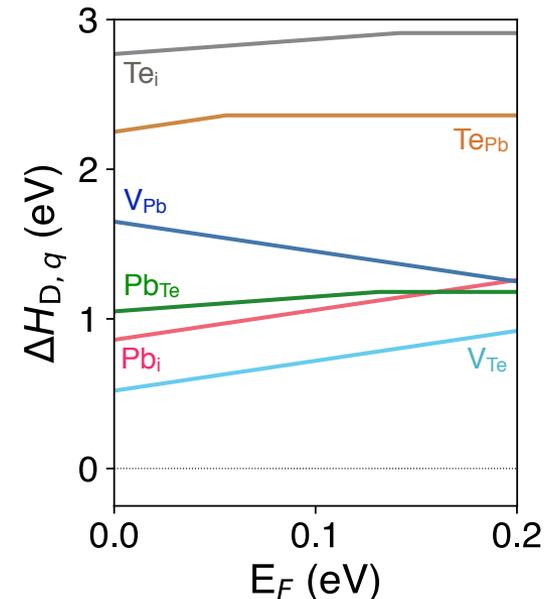
A computational framework for automation of point defect calculations

Anuj Goyal^{a,b,*}, Prashun Gorai^{a,b}, Haowei Peng^b, Stephan Lany^b, Vladan Stevanović^{a,b}

Why do we need a defect data format and repository?



Defect Diagram: Example PbTe



- The problem is two fold:
 - No standard data format for sharing defect energetics, requires cumbersome plot digitization to grab data
 - Partly due to the lack of a shareable data format, a data repository of defect calculations is missing that would otherwise be immensely useful

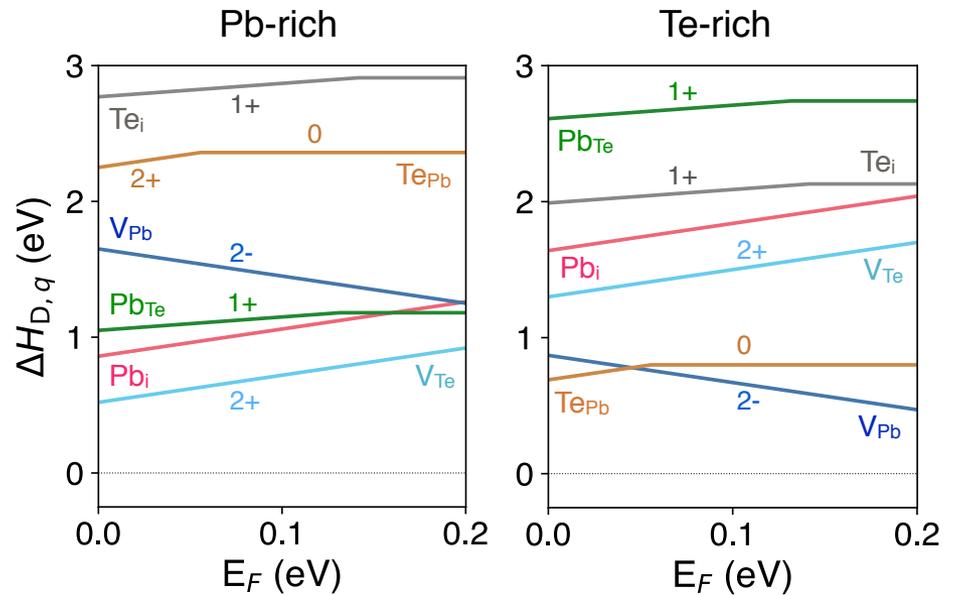
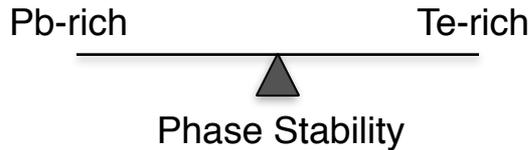
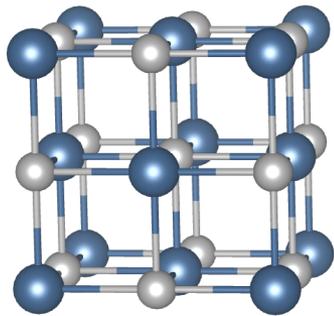
A Simple Example of a Defect Diagram: PbTe

$$\Delta H_{D,q}(E_F, \mu) = [E_{D,q} - E_H] + \sum_i n_i \mu_i + qE_F + E_{\text{corr}}$$

↓
↓
↓
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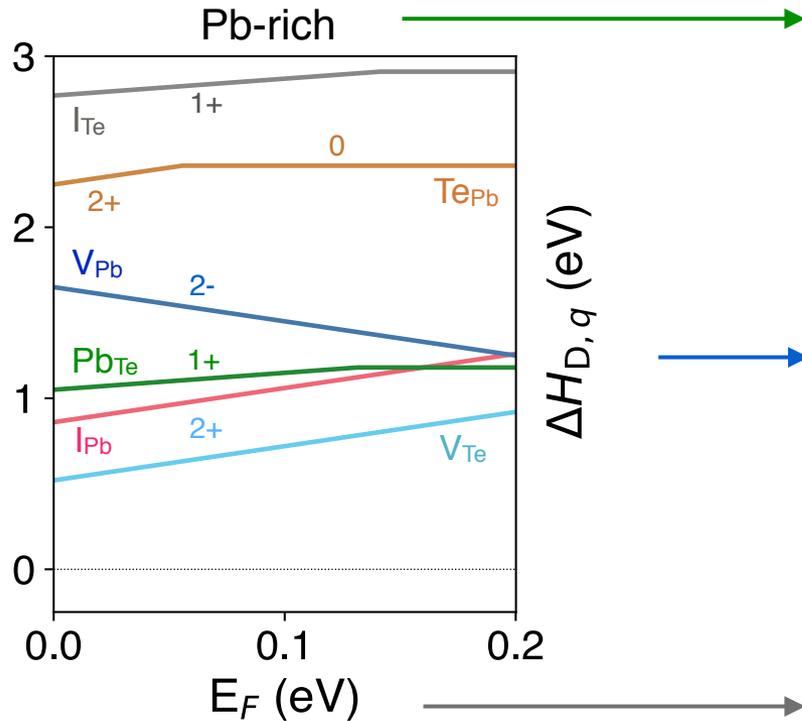
Defect Formation Energy Defect Supercell Host Supercell Chemical potentials from phase stability Electron chemical potential Finite size corrections

Rocksalt PbTe



What Should the Defect Data Format Look Like?

Defect Diagram

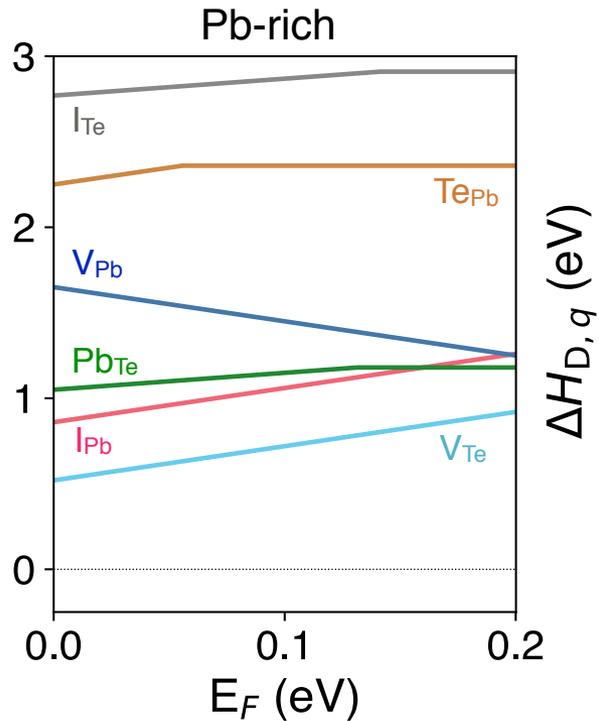


Defect Data Format

Phase Stability				
Energy	Type	Site	Charge	Label
0.52	V	Te	2	V_Te_2
0.86	I	Pb	2	I_Pb_2
1.05	Pb	Te	1	Pb_Te_1
1.65	V	Pb	-2	V_Pb_-2
2.36	Te	Pb	0	Te_Pb_0
2.77	I	Te	1	I_Te_1
Band gap				

What Should the Defect Data Format Look Like?

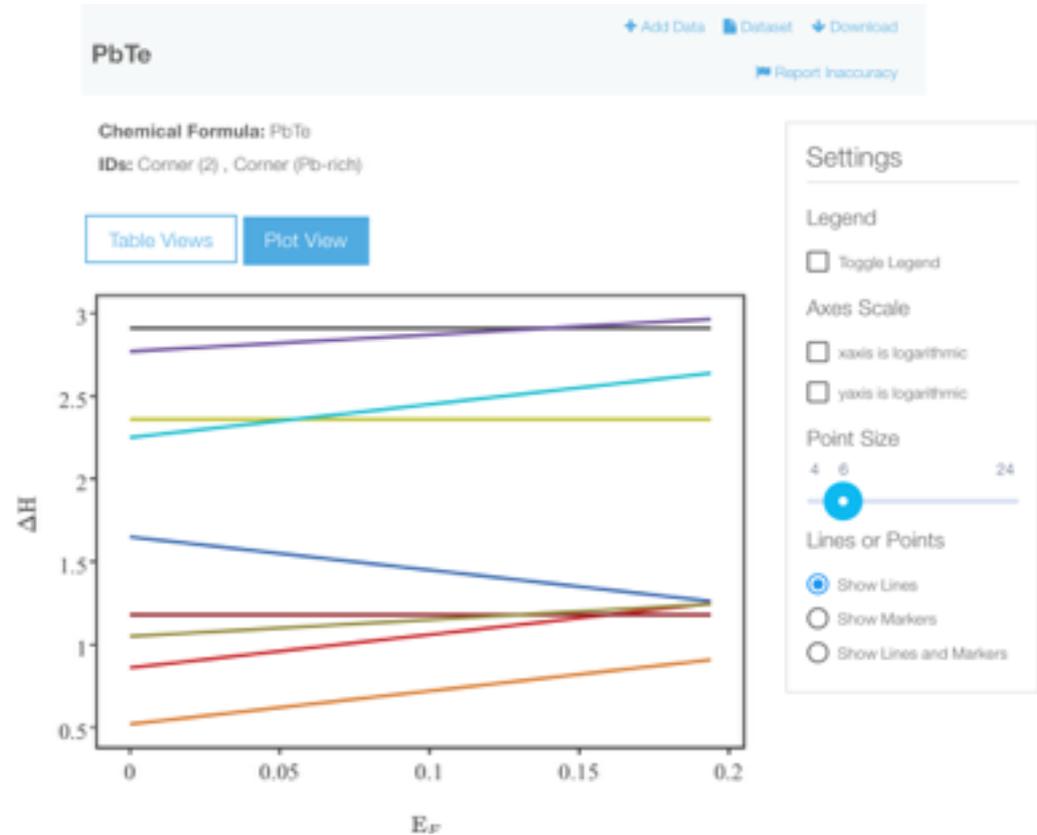
Defect Diagram



Data Format



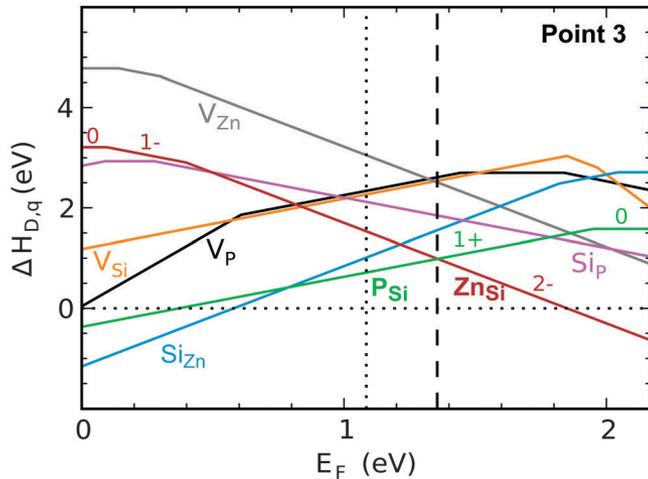
Defect Diagram



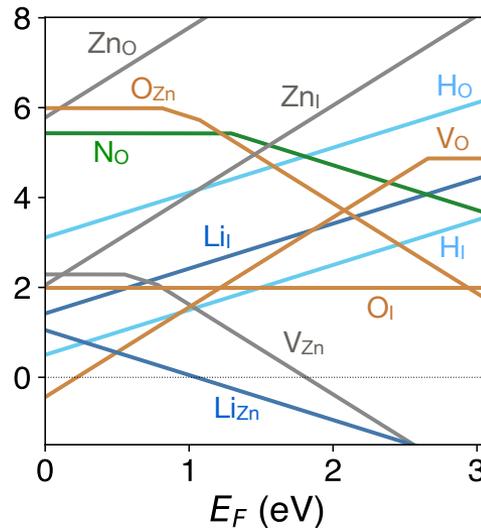
Examples of More Complicated Defect Diagrams

Defect physics of ZnSiP₂

Gorai *et al.*, Energy Environ. Sci. 9, 1031 (2016)

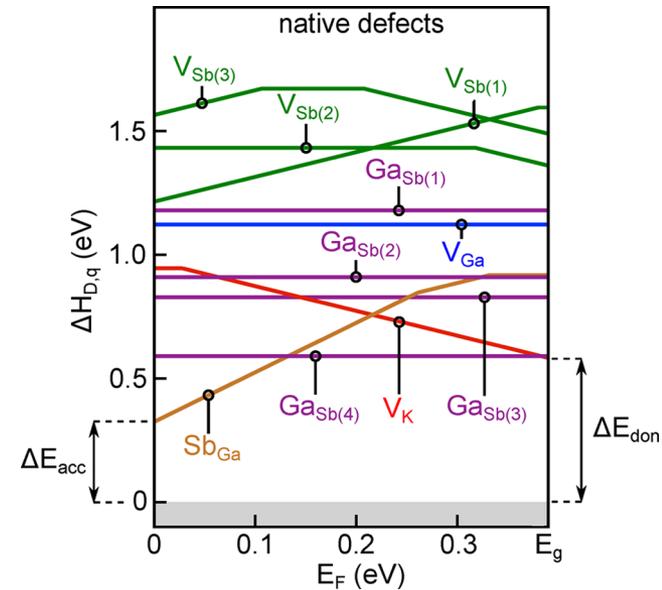


p-type doping in rocksalt ZnO



Defect Chemistry in n-type Zintl KGaSb₄

Ortiz *et al.*, Chem. Mater. 29, 4523 (2017)



- Definitely more complicated defect diagrams, but they can be reproduced using the same minimal defect data format. Check out: [Citrine Webpage](#)

Looking Ahead: Building a Public Repository

- **Test the parser** for more complicated defect diagrams
- Once parser is ready, **build a public repository** on Citrine for sharing defect diagrams
- Encourage the community to use the **data format for sharing** - example, supplementary data for publication
- Once the repository has a sizable number of materials, use **data informatics tools** on Citrine to tease out trends etc.

Thank you!