High Temperature Defects: Linking Solar Thermochemical and Thermoelectric Materials

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CSM: Vladan Stevanovic, SLAC: Michael Toney, UIUC: Elif Ertekin, NREL: Stephan Lany, David Ginley

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DMREF/EMN Kick-Off Meeting

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Award #	EE000XXXX
Year 1 Funding	$0.1M

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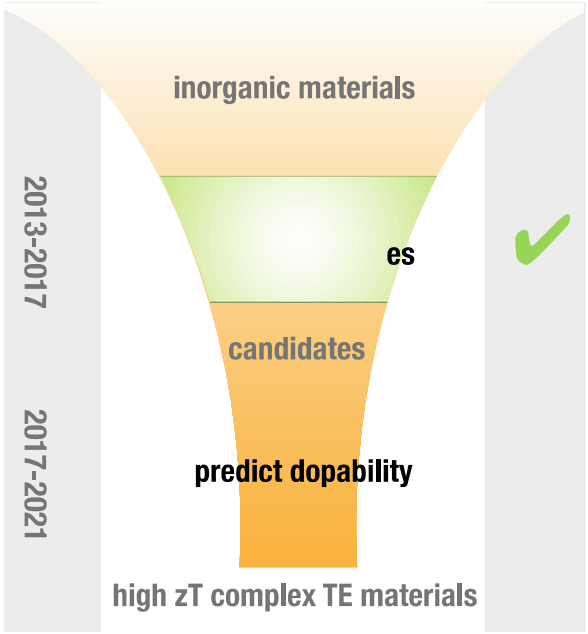
Project Vision

We are advancing our understanding of native defects (chemistry, concentration) and associated charge carriers across diverse chemistry at high temperatures.

Project Impact

Native defects can enable or “kill” materials emerging for thermoelectric and STC applications, particularly down stream in high-throughput searches.



Innovation and Objectives

Project History

NSF team has focused on developing a combined computational/experimental defects database (non-oxide materials) over the last year. NREL team has focused on oxide materials for STC.

Proposed Targets

Metric	State of the Art	Proposed
Defects database	*No publicly-available defects database*	Develop first-ever defects database
Mixed-anion defects	*Explored for PV contacts (e.g. LaCuOS), no large-scale study*	Understand defect chemistry in mixed-anion TE, STC mat.
High-T complexes	*Few examples, trial-and-error approach*	Model defect complexes in TE, STC materials

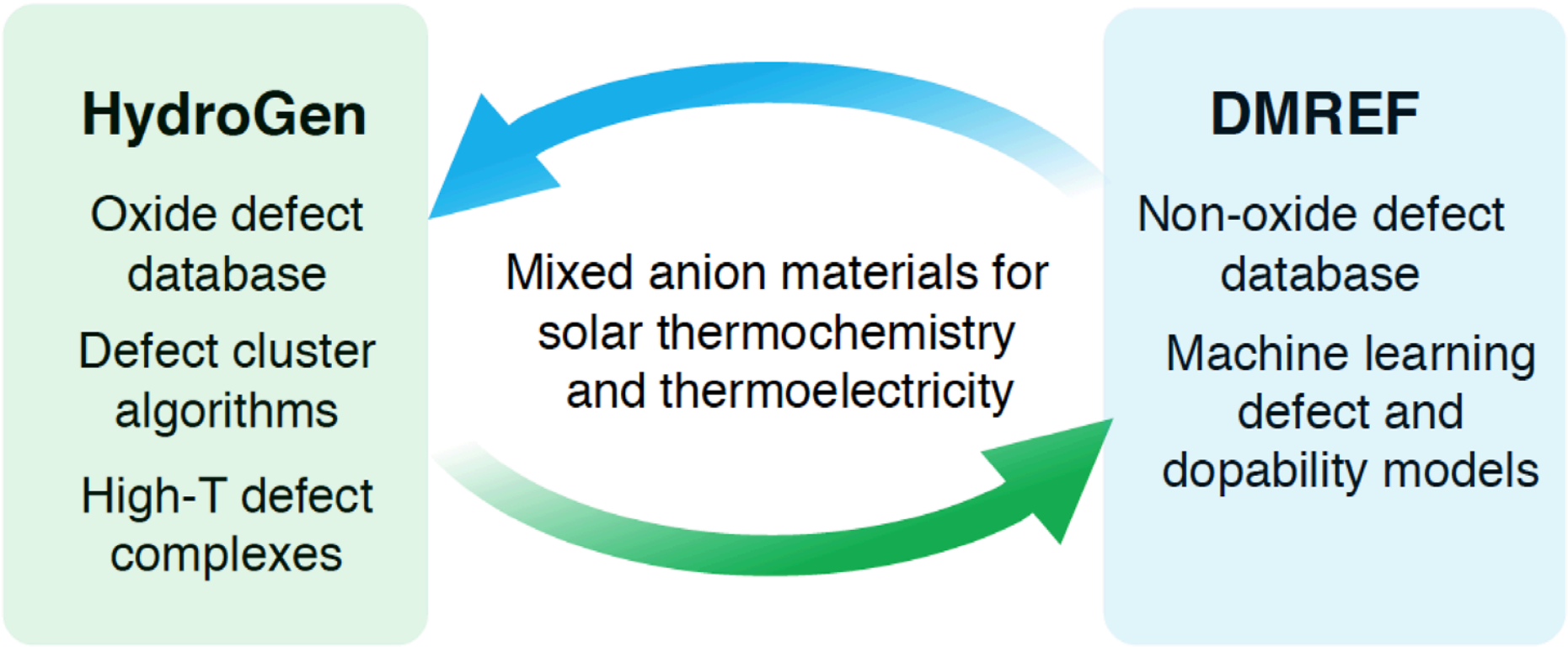
Barriers

- Development of a large defects database for trends to emerge
- Defects in mixed-anion materials
- Formation of high-T defect complexes
- Experimental validation

Partnerships

- Defects database (CSM/UIUC: non-oxides, NREL: oxides)
- Mixed-anion defects (CSM/NREL)
- High-T complexes (CSM/NREL)
- Experimental probing of local defect environments (CSM/SLAC)

Technology Innovation



Impact on water splitting:

- Increased chemical breadth enables emergence of new materials
- Underlying thermochemistry of defects and chemical/structural drivers emerge

Effective Leveraging of the EMN Resource Nodes

- Nodes utilized:
  - NREL STCH 1 - Computational and Experimental Tools for Enhanced Thermochemical Hydrogen Production
    - High-throughput computational examination of redox thermochemistry.
    - Experimental synthesis and characterization of redox oxides.
    - Dynamic STCH cycle and in-operando mechanistic and kinetic studies of redox oxides.
  - First Principles Materials Theory for Advanced Water Splitting Pathways
    - Materials screening" will utilize existing databases and high-throughput computation to perform a broader search for advanced materials with superior properties.
    - Detailed theory will address the materials physics via in-depth computational studies
- Interactions with EMN node experts to date:
  - Collaboration with Lany and Ginley on thermoelectric-focused LDRD (2013-2015)