Functional Materials by Design for Solar Energy Conversion

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Global Energy Challenge: Sustainable Materials, Processes and Systems

Sustainable development is development that meets the needs of the present without compromising the ability of future generations to meet their own needs.

– UN Bruntland Commission

- Greenhouse Gases
- Land Use
- Water Use
- Resources
- Hazards
- Waste

Integration at Scale

Cost ($/W)

Reliability

Performance
In 1898, delegates from across the globe gathered in New York City for the world's first international urban planning conference. One topic dominated the discussion. It was not housing, land use, economic development, or infrastructure. The delegates were driven to desperation by horse manure.

The situation seemed dire. In 1894, the Times of London estimated that by 1950 every street in the city would be buried nine feet deep in horse manure. One New York prognosticator of the 1890s concluded that by 1930 the horse droppings would rise to Manhattan's third-story windows. A public health and sanitation crisis of almost unimaginable dimensions loomed.

And no possible solution could be devised. After all, the horse had
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- Eric Morris, UC Davis
Numerous materials classes are vital to “Clean Energy Technologies”
Elements in the Si Microelectronics Industry –
Complexity is Increasing

FIG. 1. Increasing utilization of different elements in the silicon microelectronics industry, as a function of time. Reproduced with permission from IBM Corporation.

from Green et al. J. Appl. Phys. 113, 231101 (2013)
~30 elements

~75 elements
MGI represents a multi-faceted “Innovation Ecosystem”

From E. Miller, DOE-EERE, Dec 2014
Materials by Design provides a scientific framework to accelerate the discovery of new materials.
“Inverse Design”: Declare first the functionality you need, then use theory-guided experiment to iteratively find the material that has this target functionality.
1. Design and discover new energy-relevant materials with targeted functionalities.
2. Develop foundational theoretical, synthesis, characterization tools.
3. Incorporate functional metastable materials into MbD.
4. Develop a systematic theory-driven approach to guide synthesis.

Address four Critical Gaps limiting Materials by Design
1. Multiple-Property Design
2. Accuracy and Relevance
3. Metastability
4. Synthesizability

MIT: Alexie Kolpak, Tonio Buonassisi
Harvard: Dan Nocera, Roy Gordon
CSM: Vladan Stevanovic, Brian Gorman
NREL: Bill Tumas, Dave Ginley, John Perkins, Stephan Lany, Andriy Zakutayev

LBL: Gerd Ceder, Kristin Persson
Oregon State: Janet Tate
SLAC: Mike Toney
Two Main Approaches to Materials by Design

Design by Design Principles
- Many material systems with known structure and composition (e.g. ICSD)
- Functionality unknown
- Search via design principles for targeted functionalities

Missing Materials
- Many material systems, but structure unknown
- Many (~ 50–100) possible configurations, requiring energy minimization and stability analysis.
- Target properties: first existence, then other properties

G. Ceder, and K.A. Persson
**Tools for Materials by Design**

**Computational and Theory Tools**
- Theory (Accuracy, speed)
  - Band gaps (GW)
  - Defects
  - Heats of Formation (GGA+U)
- (Search)
  - GSGO, GA
  - High throughput platforms
  - Multiple property search

**Experimental Tools**
- Experimental (High throughput)
  - PLD, sputtering-combinatorial
  - Rapid characterization
- (Detailed Studies)
  - Bulk synthesis
  - Detailed characterization
  - Specialized structure- SLAC

**Data Management & Mining**
- Search
  - GSGO, GA
  - High throughput platforms
  - Multiple property search
Band gap prediction: **GW scheme for transition metal oxides**

- Density functional theory (DFT) is known to severely underestimate band gaps.
- **GW** problematic for *transition metal (TM) oxides*.
- Approach: **GW** with additional potential term for *d*-orbital energies (GW+V_{d})
  \[ \hat{V} = \sum_{i,j} p_i \left\langle \phi_i^{AE} V_d^{AE} \phi_j^{AE} \right\rangle p_j \]
- One empirical parameter per TM atom, good transferability, e.g., to ternaries.
- Efficient band gap prediction (semi-high-throughput) for 100s-1000s materials.

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PYLADA—end-to-end HT computational material science

Example: Programmatically chaining VASP runs:

```python
>>> calc1 = vasp1(structure, outdir='first_calculation')
>>> calc2 = vasp2(structure, restart=calc1, outdir='second_calculation')
```

Pylada is the computational “engine” behind HT computations of CID and CNGMD
Combinatorial approach

Deposit compositionally graded thin films (combinatorial libraries)

Stationary targets
Stationary substrate
Composition spread is achieved by geometry of sputter guns

Measure composition and properties as a function of position (property mapping)
NREL High-Throughput Experimental Tools

Thin Film Deposition

- 4 Dedicated PVD System
  - 3 RF sputtering
  - 1 PLD
- Composition Gradients
- Thickness Gradients
- Temperature Gradients
- Ar, N, O, Ar/H₂S gasses
- Atomic S & N sources

Property Mapping

- 15 Mapping Tools
  - Composition (XRF, RBS)
  - Structure (XRD, Raman)
  - Transport (4pp, Seebeck)
  - Optical (UV-Vis, IR, PL)
  - Surface (KP, XPS/UPS)
  - Microscopy (SEM, AFM)

Analysis & Visualization

- Advanced Data Tools
  - NREL Data Network
  - Igor PRO framework
  - Extensible
  - User-assisted analysis
  - Data mining/analysis
Combi-sputtering

Oxides

Combi PLD

Chalcogenides

from A. Zakutayev, NREL
Approach for Materials by Design

1. Define target properties
2. Articulate "Design Principles"
3. Initial selection of materials classes (each representing $10^3$-$10^6$ individual compounds)
4. Screening of promising individual candidate materials
   - High-Throughput synthesis and characterization
   - Inverse-Band-Structure search
5. Narrowed list: "Best of class"
6. Targeted synthesis and specialized characterization of candidate compounds
   - Direct materials synthesis
   - Direct theoretical characterization
   - Direct experimental characterization
7. Novel inorganic materials with tailored properties

Steps:
- Overarching design principles
- Step 1 of materials search/design
- Step 2 of materials search/design
- Final goal/outcome
Implementing Inverse Design

Designing p-Type Ternary Oxides

**DEVELOP** p-type TCO design principles

**SEARCH** $\text{A}_2\text{BO}_4$ w.r.t. design principles

**IMPROVE** Co$_2$ZnO$_4$ based on design principles
Inverse Design By Design Principles

**P-TCO PROPERTIES**

- High hole concentration (*defect calc.*)
- High hole mobility (*polaron calc.*)
- Transparency (*band-structure calc.*)

**DESIGN PRINCIPLES**

- Absence of hole-killer defect
- Presence of hole-producing defects
- Anti-bonding valence band maximum
- No bound polarons
- Optical band gap > 3 eV
- Wide ligand field splitting (some cases)

**Chose Search Space:** \( \text{A}_2\text{BO}_4 \) Spinels – 40 in ICSD
Selection of Ternary $A_2B^2O_4$ Compounds

A broad class for materials discovery

Normal 3-2 Spinels:
$A^{+3}$ $O_h$ site (e.g., Al, Fe, Co)
$B^{+2}$ $T_d$ site (e.g., Mg, Zn, Fe)

Inverse 3-2 Spinels:
$A^{+3}$ $O_h, T_d$ sites (e.g., Fe, Co)
$B^{+2}$ $O_h$ site (e.g., Ni)

• Large family of compounds
• Wide range of physical and chemical properties; low oxygen vacancy
Role of Anti-Site Defects in Spinels

Ability to calculate defects and dopants is critical to electronic materials design (supercell approach)

Anti-site defects control properties:

\[ A^{3+} \text{ on Td is DONOR} \]
\[ B^{2+} \text{ on Oh is ACCEPTOR} \]

DT-2--No Intrinsic Hole Killer !!

\[ \text{Co}_2(\text{Zn,Ni})\text{O}_4 \] – best of class!

12 of 40 $\text{A}_2\text{B}_2\text{O}_4$ Spinels Type 2 (Naturally P-Type)


Low Cost + Non-Toxic $\rightarrow$ Take $\text{Co}_2\text{ZnO}_4$ as Prototype
Three ways to improve conductivity in Co spinels:

2+ on $O_h$ site produces holes

Maximize this to increase conductivity

1. Non-equilibrium growth

2. Extrinsic dopants

3. Induce inverse spinel phase

5x improvement

20x improvement

10000x improvement
Optical and Electrical properties are optimized in a non-trivial composition region
Zn-Co-O as a hole transport layer (HTL) for OPV

- Performance comparable to PEDOT:PSS on the first try

"Zn-Ni-Co-O wide-bandgap p-type conductive oxides with high work functions"
Absorption Screening

• High Throughput screening:
  – First-principles quasi-particle GW method \( \text{G}_0\text{W}_0 + \text{HSE06} \)
  – Provides good band gap estimation

• Input:
  – ICSD structure
  – No element or stoichiometry restrictions

• Output:
  – Band gap type
  – Absorption spectra
  – Electronic structure
Developing new Metrics – Spectroscopic Limited Maximum Efficiency (SLME):

Generalized $\text{I}^{p}\text{III}^{q}\text{VI}^{r}$ chalcopyrite group

Any possible $(p, q, r)$; oxidation states of III can be 1 or 3

$(>300$ compounds$)$

$\text{CuInSe}_2, \text{CuGaSe}_2, \text{Cu(In,Ga)Se}_2$
High SLME materials include known absorbers

Other experimentally confirmed PV absorbers (less studied)

Previously unrecognized high SLME materials

**Cu-III-VI → Cu-V-VI**

<table>
<thead>
<tr>
<th>Cu-III($s^2p^1$)-VI</th>
<th>Cu-V($s^2p^3$)-VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al (3+)</td>
<td>P (5+, 3+)</td>
</tr>
<tr>
<td>Ga (3+)</td>
<td>As (5+, 3+)</td>
</tr>
<tr>
<td>In (3+)</td>
<td>Sb (5+, 3+)</td>
</tr>
<tr>
<td>Tl (3+, 1+)</td>
<td>Bi (5+, 3+)</td>
</tr>
</tbody>
</table>

**Low valence compound:** Cu-V(3+)-VI  
**High valence compound:** Cu-V(5+)-VI
Case of Cu-Sb-S: 
**Cu-Sb\(^{3+}\)-S vs. Cu-Sb\(^{5+}\)-S vs. CuInSe\(_2\) (CIS)**

Both Cu\(_3\)SbS\(_3\) and CuSbS\(_2\) have stronger absorption than Cu\(_3\)SbS\(_4\) and CIS for \(h\nu > E_g + \Delta\).

\(\Delta\) depends on the energy difference between indirect gap and direct gap

- CuSbS\(_2\): 0.05 \((E_g^d - E_g^i)\)
- Cu\(_3\)SbS\(_3\): 0.13 \((E_g^d - E_g^i)\)

- Increase p DOS near CBM and s DOS near VBM

Perovskite Electronic Structure (MAPbI₃)

- Perovskite cage filled with dipolar cation
- Excellent transport properties:
  - Minority carrier diffusion lengths > 1μm in thin films, 175μm in single crystals
  - Monomolecular recombination lifetimes of 280 ns
  - Minority carrier mobilities ~ 10 cm²/V/s are reasonable

- Design Criteria

**Design Criteria**

\[ \varepsilon_r \quad m^* \quad \text{Antibonding VBM, Bonding CBM} \]

Two Main Approaches

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Missing Materials
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G. Ceder, and K.A. Persson
Missing Materials Search
Challenge 1: Structure of an unknown compound

General solution:
Global Space Group Optimization (GSGO)

Alternative:
- 39 structures-types for 800 known $A_2B\text{X}_4$
- GGA+U to sort out the ground-state structure

<table>
<thead>
<tr>
<th>No.</th>
<th>Name (example)</th>
<th>Space Group</th>
<th>Occurrence</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Spinel ($\text{Al}_2\text{MgO}_4$)</td>
<td>Fd3m</td>
<td>255</td>
</tr>
<tr>
<td>2.</td>
<td>NN ($\text{Th}_3\text{P}_4$)</td>
<td>I43d</td>
<td>87</td>
</tr>
<tr>
<td>3.</td>
<td>Olivine ($\text{Al}_2\text{BeO}_4$)</td>
<td>Pnma</td>
<td>48</td>
</tr>
<tr>
<td>4.</td>
<td>Hausmanite ($\text{Mn}_3\text{O}_4$)</td>
<td>I4/amd</td>
<td>27</td>
</tr>
<tr>
<td>5.</td>
<td>Phenakite ($\text{Li}_2\text{WO}_4$)</td>
<td>R3</td>
<td>14</td>
</tr>
</tbody>
</table>

...
High - Throughput calculations

Scope:
• 406 $A_2BX_4$
• 39 structure-types for each $A_2BX_4$
• Several magnetic configurations

Software development:
1) Setting up automatically the crystalline and magnetic structure for each potential ground state
2) Automatic detection of errors
3) Automatic extraction of properties

~80 000 GGA+U calculations
~$10^6$ CPUh
Missing Materials Search
Challenge 2: Stability with respect to competing phases

$$\Delta H_f(A_m B_n X_l) = E_{\text{tot}}(A_m B_n X_l) - (m\mu_A^0 + n\mu_B^0 + l\mu_X^0)$$
Illustration of the DFT failure

- 45 binary pnictides and chalcogenides of 3d transition metals
- Experimental $\Delta H_f$ from Thermochemical Tables (1982) and Kubaschevsky (1983)
Our approach: Fitted Elemental Reference Energies (FERE)

\[ \Delta H_f(A_mB_n) = E_{\text{tot}}^{\text{GGA+U}}(A_mB_n) - (m \mu^0_A + n \mu^0_B) \]

Fix No. 1:
GGA+U for compound total energies

Fix No. 2:
\( \mu^0 \) fitted to a set of measured \( \Delta H_f \)
(Lany, PRB, 2008)

• Underlying assumption:
\[ \delta (\Delta H_f) = \sum_i n_i \delta \mu_i \]

Same for all compounds!
Fitted Elemental Reference Energies – FERE

50 $\mu^0$ values fitted using measured $\Delta H_f$ values of 252 binary pnictides, chalcogenides and halides

$\mu^0 \text{(FERE)} = \mu^0 \text{(GGA+U)} + \delta \mu^0 \text{(FERE)}$

FERE reduces the mean average error (MAE) to 0.054 eV/atom ≈ 1 kcal/mol.

FERE Validation - Ternaries

55 ternary compounds with measured $\Delta H_f$

MAE = 0.048 eV/atom

Compound stability from FERE – Mn$_2$SiO$_4$

**Theory:**
Structure: Olivine
$\Delta H_f = -2.53 \text{ eV/atom}$

**Experiment:**
Structure: Olivine
$\Delta H_f = -2.56 \text{ eV/atom}$
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Competing phases:
Mn, Si, O$_2$
MnO
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**Experiment:**
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Competing phases:
- Mn, Si, O$_2$
- MnO, MnO$_2$, Mn$_2$O$_3$
- Mn$_3$O$_4$, SiO$_2$
Compound stability from FERE – Mn$_2$SiO$_4$

**Theory:**
Structure: Olivine
$\Delta H_f = -2.53$ eV/atom

**Experiment:**
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Competing phases:
- Mn, Si, O$_2$
- MnO, MnO$_2$, Mn$_2$O$_3$
- Mn$_3$O$_4$, SiO$_2$
- MnSiO$_3$, Mn$_4$SiO$_7$
- Mn$_5$Si$_3$O$_{12}$

Finch *et al.*

$T = 1600$ K, $p_{O_2} = 10^{-10}$ atm

$\rightarrow \Delta \mu_O = -3.45$ eV
**Theory:**
Structure: Olivine
$\Delta H_f = -2.53 \text{ eV/atom}$

**Experiment:**
Structure: Olivine
$\Delta H_f = -2.56 \text{ eV/atom}$
High-throughput Discovery of New $A_2BX_4$ Compounds

Rules:
1. only one transition metal at a time
2. respect possible oxidation states

Total 656 possible combinations
250 are reported
406 are not reported ("missing compounds")
Predicted New $A_2BO_4$

Out of 63 missing oxides
46 not stable
17 stable

Newly predicted:
- $Hg_2SiO_4$
- $In_2HgO_4$
- $Ti_2BeO_4$
- $Ti_2SrO_4$
- $Ti_2BaO_4$
- $Ti_2ZnO_4$
- $V_2BeO_4$
- $V_2SiO_4$

$A_2BX_4$ search:
~80000 individual total-energy calculations
(incl. structures and magnetic configurations)

7 already predicted by Hautier et al., Chem. Mater., 2010
Results – Sulfides

We predict:

- $\text{Hg}_2\text{GeS}_4$
- $\text{Al}_2\text{TiS}_4$
- $\text{Al}_2\text{VS}_4$
- $\text{Al}_2\text{CoS}_4$
- $\text{Al}_2\text{NiS}_4$
- $\text{In}_2\text{VS}_4$
- $\text{Sc}_2\text{BaS}_4$
- $\text{Ti}_2\text{MgS}_4$

Out of 92 not reported:
- 34 stable
- 1 undermined
- 57 not stable

---

We predict:

- $\text{Hg}_2\text{GeS}_4$
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- $\text{Ti}_2\text{MgS}_4$

---

Stevanovic et al.
CID Predicted Ternary Materials

$A_2BX_4$ materials main group and 3d elements:
Out of 684 variations, 429 are unreported
100 predicted stable, 11 undetermined, and 318 predicted not stable


ABX materials with 8 electrons:
Out of 714 variations, 488 are unreported
235 predicted stable, 18 undetermined, and 235 predicted not stable

The symmetry of a predicted stable compound makes possible:

1) Simulation of diffraction pattern

2) Fast identification in the experimental pattern

HfIrSb, ZrRhBi, ScRhTe, TaCoSn, TaIrGe, VIrSi, VRhSi and HfRhP have been shown to crystallize in their predicted crystal structure.

Example: HfIrSb

F-43m

Identifcation of ABX ternary materials

With Confirmation By Electron diffraction

Fast identification in multiphasic sample

X. Zhang et al. Nature Materials
Missing TaCoSn Compound

Not known in ICSD or ICDD

Large stability range

Predicted to have semi-conducting gap $\sim 1.3$ eV (GGA + U)

Competing phases:
- Ta, Co, Sn
- Ta$_3$Sn, TaSn$_2$
- CoSn, CoSn$_2$, CoSn$_3$, Co$_3$Sn
Validation: growth of new TaCoSn

Predicted Structure

TaCoSn Grown

XRD: Predicted & Measured

NREL materials Database http://materials.nrel.gov

High-throughput calculations

DFT level (atomic structure and total energy)
ca. 20,000 crystalline ordered materials
- Repository of atomic and magnetic structures
- Thermochemistry and stability

GW level (electronic structure)
ca. 250 semiconducting and insulating materials
- So far: Mostly oxides, chalcogenides, nitrides
- Direct and indirect band gaps
- Band-edge shifts wrt DFT (defects, IP/EA, band offsets)
- Effective masses, density of states
- Absorption spectra, dielectric function

Example:
Cu₂O band-structure and absorption
MATERIALS PROJECT

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Register now for free, full access.

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- Up to 500 search results
- History of your searches and analyses

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- 10 minute usage limit
- Search results limited to 10 best matches
- Just click an app to start

Materials Explorer
Search for materials information by chemistry, composition, or property.

Lithium Battery Explorer
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

Crystal Toolkit
Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.

Phase Diagram App
Computational phase diagrams for closed and open systems. Find stable phases and study reaction pathways.

Reaction Calculator
Calculate the enthalpy of tens of thousands of reactions and compare with experimental values.

Pourbaix Diagrams
Generate Pourbaix Diagrams from experimental ion data

Find out more about our open Materials API and pymatgen library for querying large amounts of data.

www.materialsproject.org
ICSD database and metastability

Number of new compounds entered into ICSD database by year that are ground states (green) or metastable (blue).

G. Ceder, and K.A. Persson
Incorporating Metastability into Materials by Design for Inorganic Semiconductors

1) Polymorphism
2) Defects, disorder, and interfaces
3) Semiconductor alloys

Addressing Synthesis: Provide guidance on stability and process space for materials synthesis through *in-situ* and atomistic measurement methods to elucidate the mechanisms of growth and benchmark theoretical models.

Classes of metastable materials (shown in color) targeted for theory-driven synthesis in the CNGMD EFRC.
Incorporating Metastability into Materials by Design

Classes of metastable materials (shown in color) targeted for theory-driven synthesis in the CNGMD EFRC.

- Polymorphs & Synthesizability ($\text{V} \text{O}_x$, $\text{MnO}_x$, ...)
- Ternary Pnictides Search (Sn-Ti-N)
- Tin Chalcogenide Alloys
- Defect Phase Diagrams ($\text{Sn:Ga}_2\text{O}_3$)
Why? Materials design into metastable space will lead to multi-fold increase of possible interesting compounds

What do we know? Low energy is “required” but not “sufficient”
Approach

Theory:
- Tools to systematically investigate energy landscape around the ground states
- Develop nucleation theory in different environments (thin film, solution)

Experiment:
- Solution and vapor phase growth of materials
  - Electrochemical, hydrothermal
  - PLD, PVD, PVD
- Ex-situ and in-situ characterization

Substrate and growth parameter dependence
SLAC: In-situ crystallization of amorphous films

Deposition → Amorphous films → Crystallization

X-rays
**Systems: MnOx, VOx**

**MnO_x**: over 30 known polymorphs known: batteries, catalysts, …

**VO_x**: high polymorphism and high technological relevance

- beta
- ramsdellite
- alpha
- delta
- lambda

- Columbine
- Anatase
- Rutile
- A-Phase
- B-Phase

**Columbine**, **Anatase**, **Rutile**, **A-Phase**, **B-Phase**
**Polymorph sampler – energetics**

**Scientific Objective:** Create a first-principles-theory based high-throughput computational tool to predict the formation energy and functionality of polymorphs including new unknown structures.

Local DFT relaxations on a large set of random superlattices (RSL) with quasi-random atom distribution on the RSL planes to promote realistic cation-anion coordination.
"Phase Space" likely matters too

- Both the width and depth of the basins of attractions are relevant
- Width measures the probability to get into a certain structure, while depth measures the kinetic barrier
Measuring the “width” of basins of attraction

“Let it rain and measure how much water there is in each well”

“Rain” → random sampling
Rel. Freq. of Occurrence of a given structure measures the “amount of water”

Local DFT relaxations on a large set of random superlattices (RSL) to bias sampling to cation-anion coordination
- 1,000 RSLs constructed and fully relaxed using standard DFT/GGA
Test Cases: MgO, ZnO, SnO$_2$

The occurrence frequency in RSL sampling is a measure for the basin of attraction size, i.e. the probability of “falling” into a given structure. All observed polymorphs of MgO, ZnO and SnO$_2$ are shown to be the top occurring structures in agreement with experiment.
Design of semiconducting tetrahedral Mn$_{1-x}$Zn$_x$O alloys for water-splitting

Metastable transition metal oxide alloy with unique semiconducting properties

- Band gap control through alloying
- Non-equilibrium growth via PLD
- PEC measurements
  - Band alignment, carrier transport

Measured absorption coefficient $\alpha$ (contour plot) and calculated band gaps (dashed line) (H. Peng, P. Ndione, D.S. Ginley, A. Zakutayev, S. Lany, Phys. Rev. X 5, 021016 (2015))
Brief Summary: Materials by Design

Materials by Design has advanced considerably
  - Number of active centers
  - Structural and functional materials
  - Tools being developed
  - Workflows, data generation, data curation, data mining
  - Extensive databases being developed

Integration (and iteration) of theory and experiment is critical
  - Tool development
  - Validation, accuracy

Materials Properties for have been predicted and confirmed

New materials have been predicted and synthesized

Computational databases are becoming readily available, applied research can be built on top of these more basic science efforts

Theory and experiment can provide information on metastable systems, e.g. polymorphs
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## Acknowledgements: CID EFRC

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<tr>
<th>Partner</th>
<th>Senior Investigators, <em>Staff and Students, Graduates/Alumni</em></th>
</tr>
</thead>
<tbody>
<tr>
<td>NREL</td>
<td><strong>Dave Ginley, John Perkins, Stephan Lany, Andriy Zakutayev, Peter Graf, Jun Wei Luo,</strong> <em>Paul Ndione, Haowei Peng, Vince Bollinger, Josh Martin,</em> Mayeul d’Avezac, Alberto Franceschetti, Arkadiy Mikhaylushkin</td>
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<tr>
<td>Northwestern University</td>
<td><strong>Ken Poeppelmeier, Art Freeman, Tom Mason, Giancarlo Trimarchi, Feng Yan, Arpun Nagaraja, Jimo Im, Kanber Lam, Romain Gautier, Kelvin Chang, Jeremy Harris, Karl Rickers,</strong> Evan Stampler, Nicola Perry, Veerle Cloet, Adam Raw</td>
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<tr>
<td>Oregon State University</td>
<td><strong>Doug Keszler, John Wager,</strong> <em>Robert Kokenyesi, Jae-Seok Heo, Greg Angelos, Brian Pelatt, Ram Ravichandran,</em> Jeremy Anderson, Vorranutch Jieratum, Ben Waters, Emmeline Altschul</td>
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<tr>
<td>University of Colorado - Boulder</td>
<td><strong>Alex Zunger, Liping Yu,</strong> Lijun Zhang, <em>Josh Ford</em></td>
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<td>SLAC</td>
<td><strong>Mike Toney, Linda Lim, Kevin Stone, Yezhou Shi,</strong> Joanna Bettinger</td>
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<td>Colorado School of Mines</td>
<td><strong>Vladan Stevanovic,</strong> Xiuwen Zhang</td>
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