Materials Genomics

Trends in Nanomanufacturing: "Advances in Modeling Nanomanufacturing Processes"

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…the process of engineering matter into new useful forms*

* G. Ceder and K. Persson, Scientific American, Dec 2013

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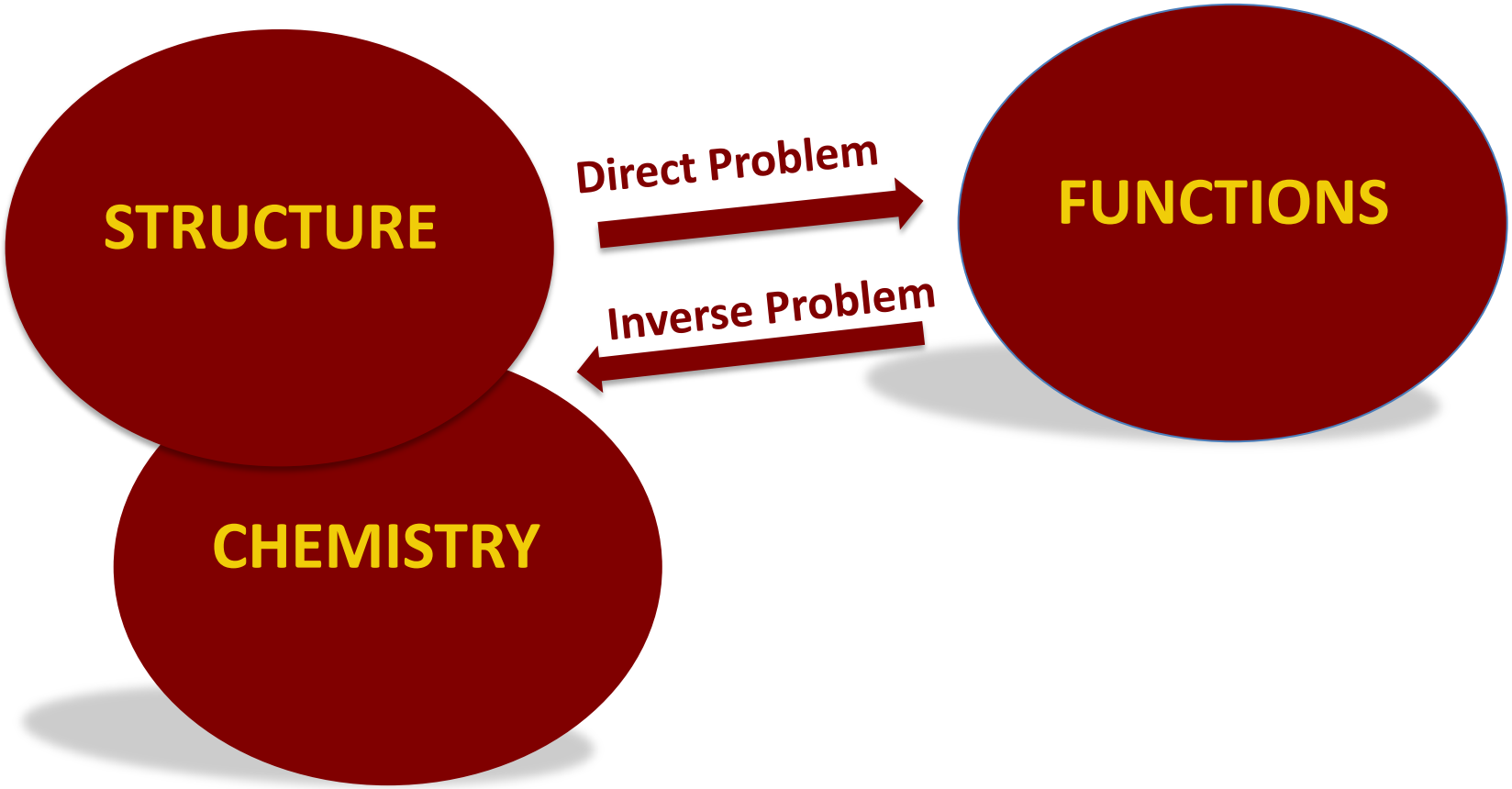

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Direct problem:

(D1) Development of methodologies to compute (measure) directly the property of interest. Application of such methodologies to selected cases.

e.g. optimized exchange-correlation functionals, non-adiabatic processes, theoretical spectroscopies, faster algorithms, improved hardware, etc.

(D2) Search for design-rules/**descriptors** for the property of interest in selected cases to provide structure (hopefully quantitatively) to the intuition.

Descriptors discovery

- ❑ Thinking
- ❑ High-throughput methodologies + Data-mining tools

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Inverse problem:

(I1) Exploration of a large configuration space by determining the property of interest and screening for optimal materials. 2

e.g. Stability of Pt-group alloys by Hart et al., Physical Review **X** (2013)

(I2) Exploration of a restricted configuration space in which property descriptors are expected to be reliable. Validation.

The real test of understanding is prediction*

3

e.g. Pb-free piezoceramics by Armiento et al., Physical Review **B** (2011/3)

1

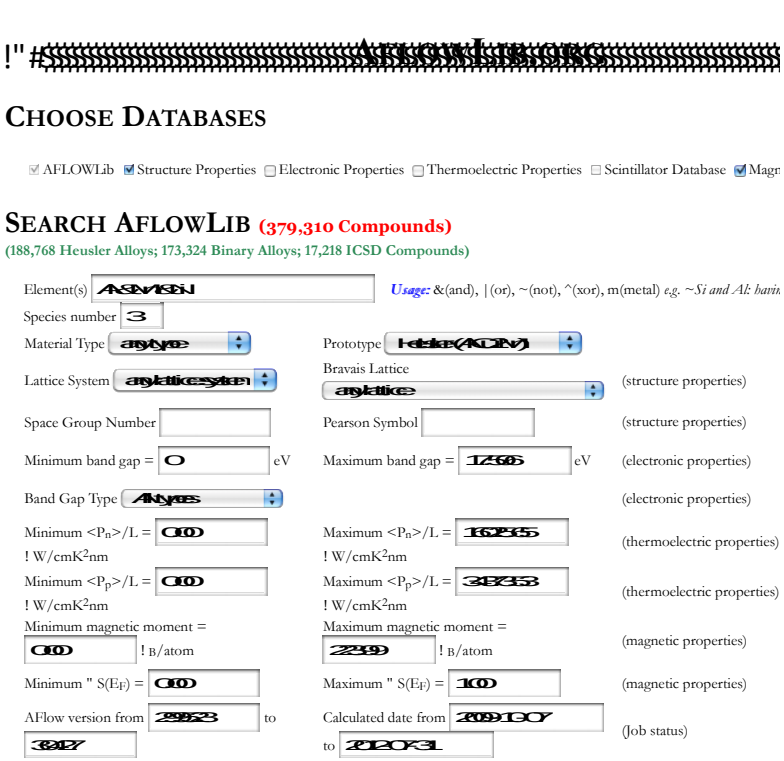
Infrastructures

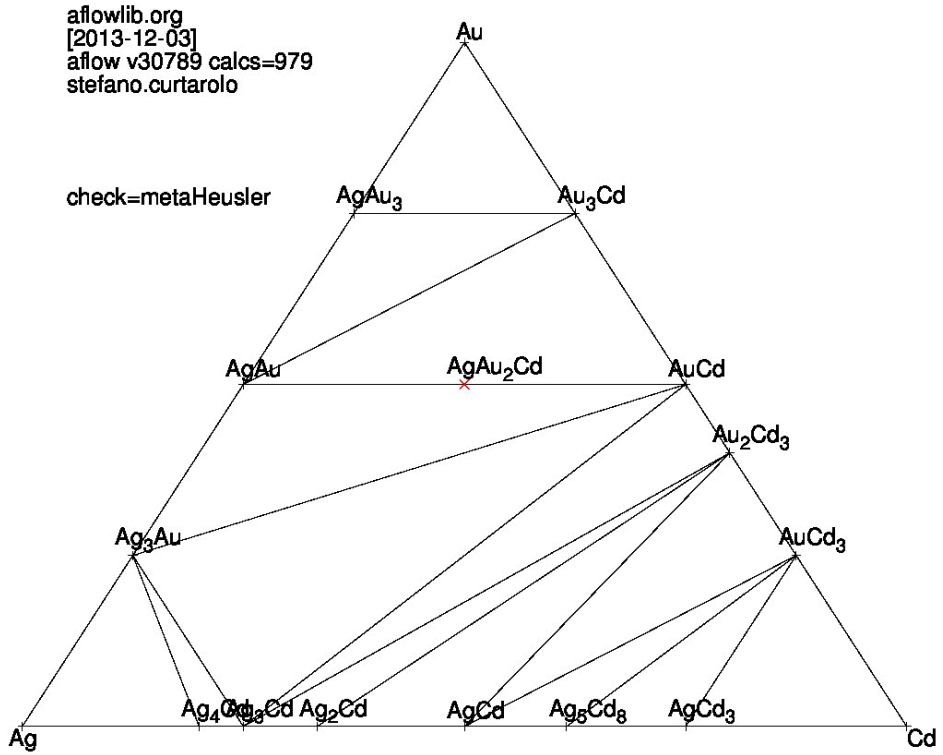
- AFLOW http://aflowlib.org

* R. Hoffmann, Solids and surfaces (VHC, 1988)

Infrastructors: AFLOWLIB Repository

- Database of DFT calculations
- > 500,000 compounds
- Online/socket commands for the SQL database interrogation.
- Distributed platform will work on Linux/UNIX platforms





Curtarolo et al., Comp. Mat. Sci. **58**, 227-235 (2012) and www.aflowlib.org

Automatic Generation of Databases

Creating “aflow.in” input files:

```
kesong@beta:/tmp$
```

HT Computational Tools (AFLOW)

+

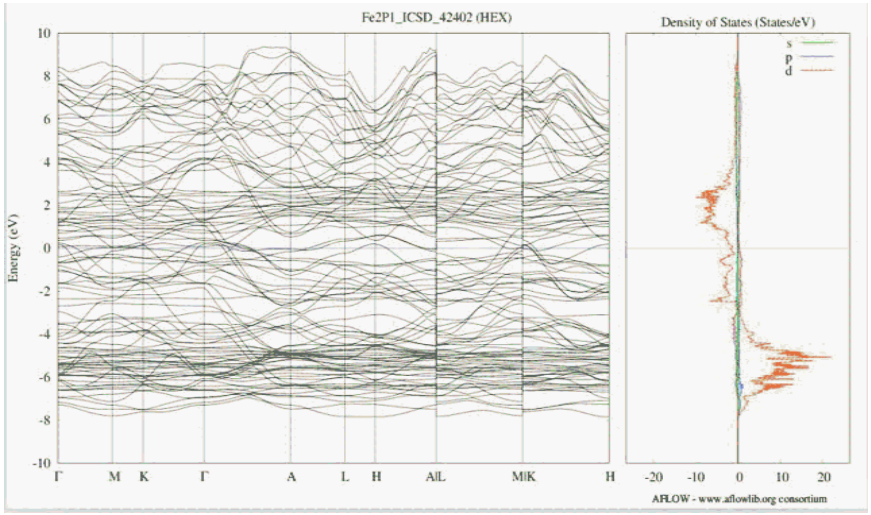
VASP/QE

Materials Database (AFLOWLIB)

Automatic data/visualization analysis

Extract general materials properties: structural, electronic, magnetic properties…

```
kesong@nietzsche:~/Example/Fe2P1_ICSD_42402$
```



Develop new high-throughput programs based on the desired materials properties

Pt-group alloys

Selected for a Viewpoint in *Physics*
PHYSICAL REVIEW X **00**, ()

Comprehensive Search for New Phases and Compounds in Binary Alloy Systems Based on Platinum-Group Metals, Using a Computational First-Principles Approach

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[2]*Center for Materials Genomics and Department of Mechanical Engineering and Materials Science, Duke University, Durham, North Carolina 27708, USA*
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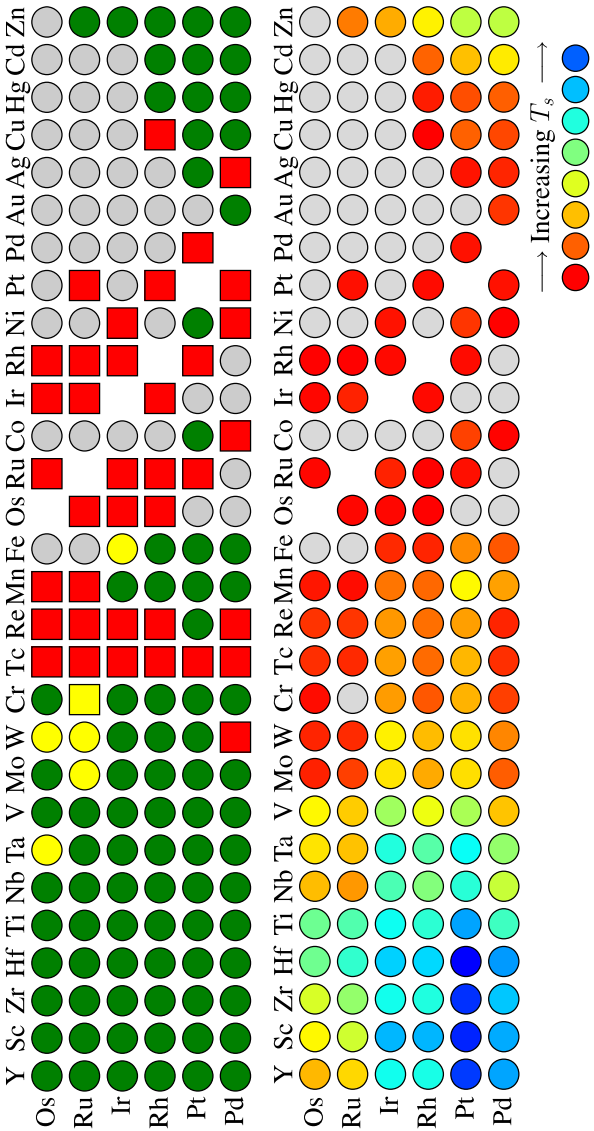
(Received 25 August 2013)

We report a comprehensive study of the binary systems of the platinum-group metals with the transition metals, using high-throughput first-principles calculations. These computations predict stability of new compounds in 37 binary systems where no compounds have been reported in the literature experimentally and for a few dozen of as-yet unreported compounds in additional systems. Our calculations also identify stable structures at compound compositions that have been previously reported without detailed structural data and indicate that some experimentally reported compounds may actually be unstable at low temperatures. With these results, we construct enhanced structure maps for the binary alloys of platinum-group metals. These maps are much more complete, systematic, and predictive than those based on empirical results alone.

DOI: Subject Areas: Computational Physics, Materials Science



- ❑ 153 binaries: prototypes+hypothetical
- ❑ Formation enthalpy: convex hull
- ❑ Competition with disorder: T_s
- ❑ 37 new phases (**@nanoscale?**)

Descriptors discovery

Table 1| Examples of descriptors introduced in the literature. Nature Mater. **12**, 191 (2013)

Problem	Combination of materials properties (gene)	Descriptor
Structure stability: convex hull of an alloy system	Formation enthalpy (H_f) as a function of concentration (x) and the enthalpies (H) of A and B.	$H_f(x) = H(A_{1-x}B_x) - (1-x)H(A) - xH(B)$
Phase stability in off-lattice alloys PRL **91**, 135503 (2003)	Spectral decomposition of alloy vector-energies ($E_{n,p}$, n-rows = species, p-columns = configurations) with principal-component-analysis coefficients (α_i) and truncation error ($\epsilon(d)$) (ref. 3).	$E_{n,p} \simeq \alpha_1 E_{n,1} + \cdots + \alpha_{p-1} E_{n,p-1} + \epsilon(d)$
Nano PR	Ratio of the av) (ref. 15).	
Topol Natu	Variational rat rbit derivative stra s at k, a_0 lattice)[16].	
Powe (spec ncy) PR	Ratio of the m ident solar energy density on–hole recombinatio E)) — versus bandgap energy (E_g)[62].	
Non-proportionality in scintillators IEEE Trans. Nucl. Sci. **56**, 2989 (2009)	Maximum mismatch between effective masses of electrons (m_e) and holes (m_h)[75].	$\hat{\chi}_{np} \equiv \max\left(\frac{m_e}{m_h}, \frac{m_h}{m_e}\right)$
Morphotropic phase boundary piezoelectrics PRB **84**, 014103 (2011)	Energy proximity between tetragonal, rhombohedra and rotational distortions (ΔE_p). Angular coordinate (α_{AB}) of the energy minimum in the A–B off-centerings energy map for ABO_3 systems[79].	$\Delta E_p \leq 0.5$ eV $\alpha_{AB} \approx 45°$

the property

qualitative descriptor

quantitative descriptor

nature materials

REVIEW ARTICLE

PUBLISHED ONLINE: 20 FEBRUARY 2013 | DOI: 10.1038/NMAT3568

The high-throughput highway to computational materials design

Curtarolo*, Hart, Buongiorno Nardelli, Mingo, Sanvito, Levy

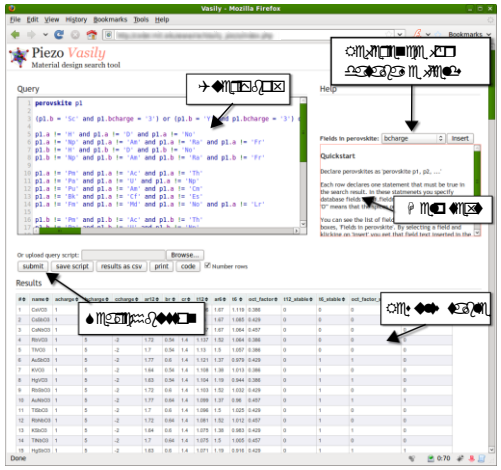
DOI: 10.1038/NMAT3568 (March 2013)

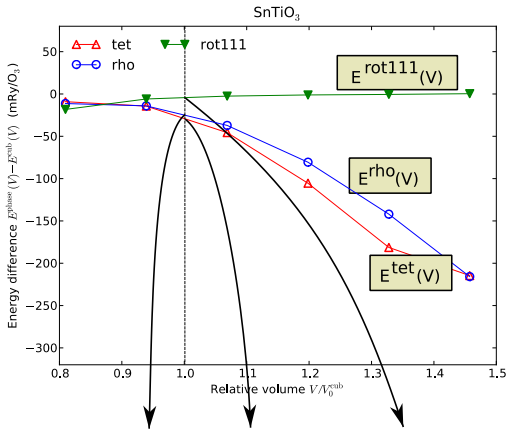
Descriptors discovery: piezoceramics

- Prototype: $Pb(Zr,Ti)O_3$ (PZT)
- ABO_3 ceramics with perovskite-like structure: 3669 compositions (up to Bi)

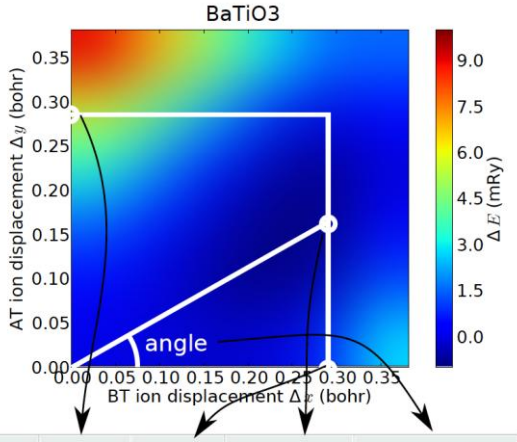
- Tetragonal Pb-free perovskite (to replace $PbTiO_3$)
- MPB forming alloys

C0: Electronic structure (insulating with d-p hybridization)
C1: Coexistence of several polar phases (RHO, TET)
C2: Competition with octahedral rotations/tiltings
C3: Large A-/B-site interplay





name	energy_rel_cubvol_rho_PBE	energy_rel_cubvol_tet_PBE	energy_rel_cubvol_rot111_PBE
SnTiO3	-0.310343	-0.340953	-0.058061



name	landscape_at	landscape_bt	landscape_atbt_min	landscape_atbt_min_angle
BaTiO3	0.043468	-0.002162	-0.01336	0.22043186

Descriptors application: piezoceramics

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C1: Coexistence of several polar phases (RHO, TET)
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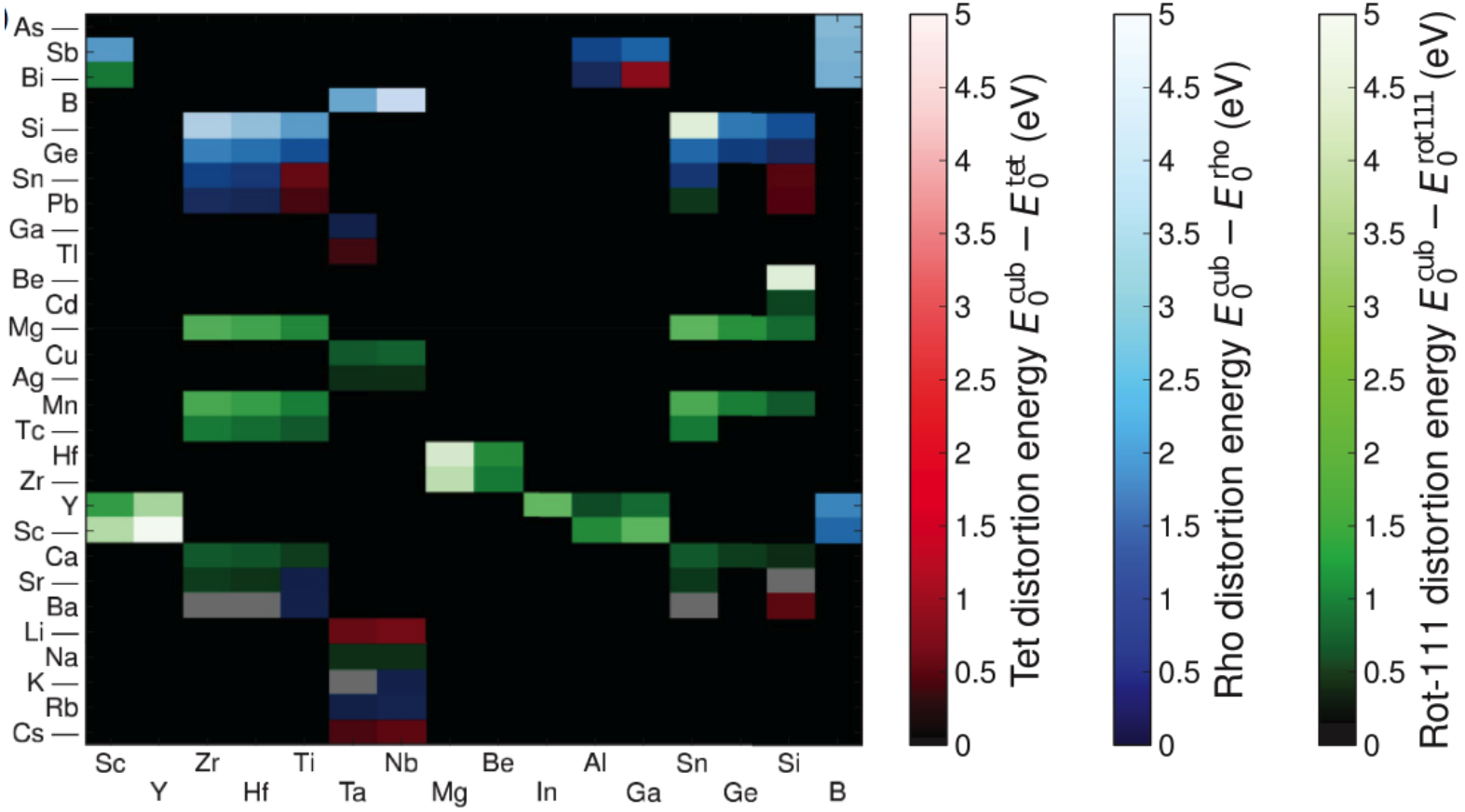

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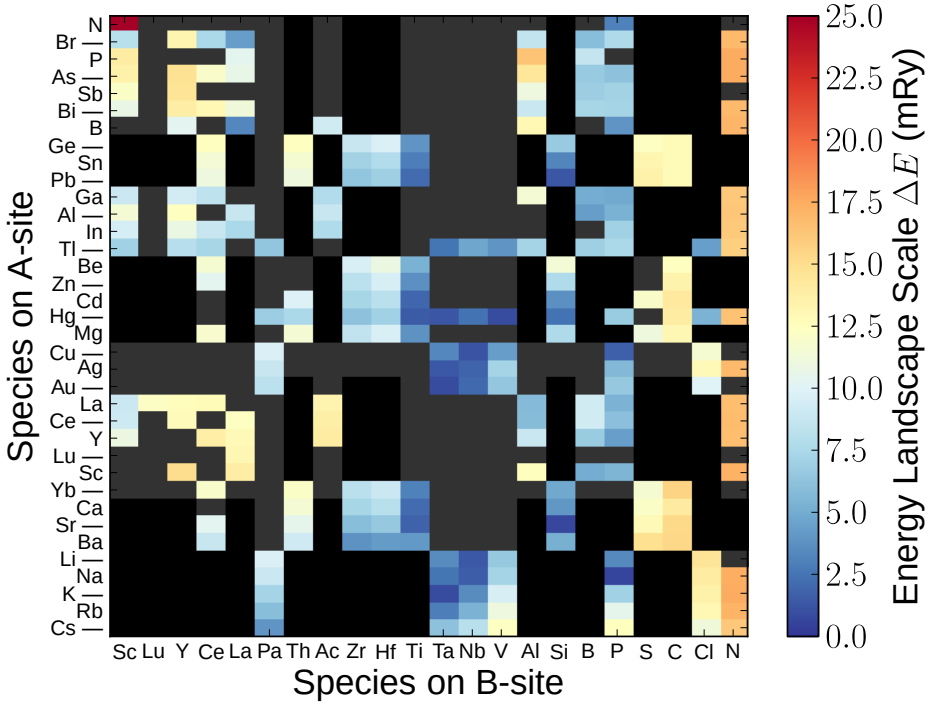
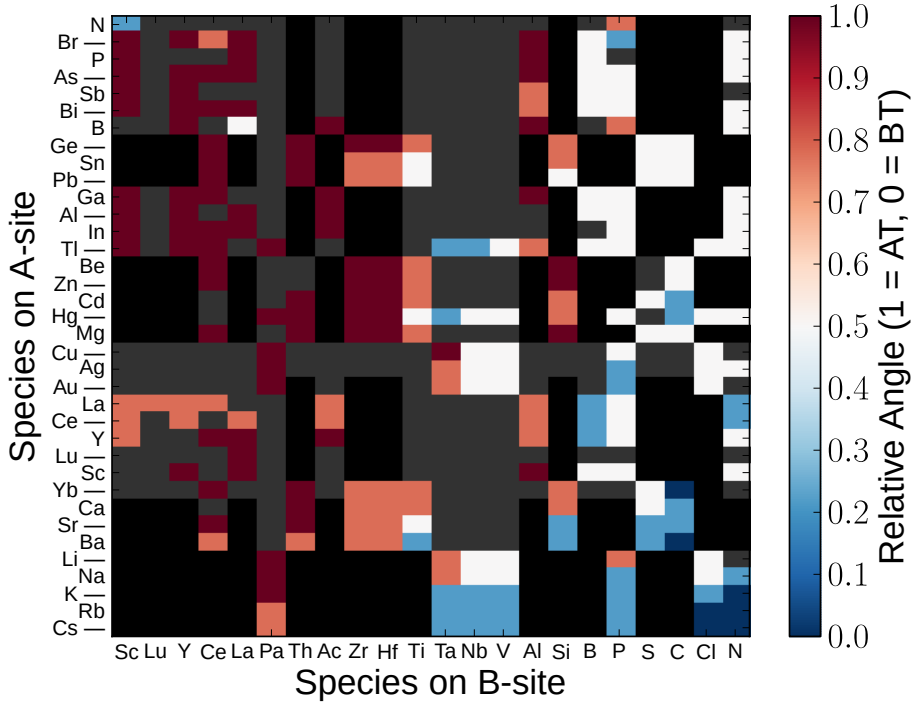
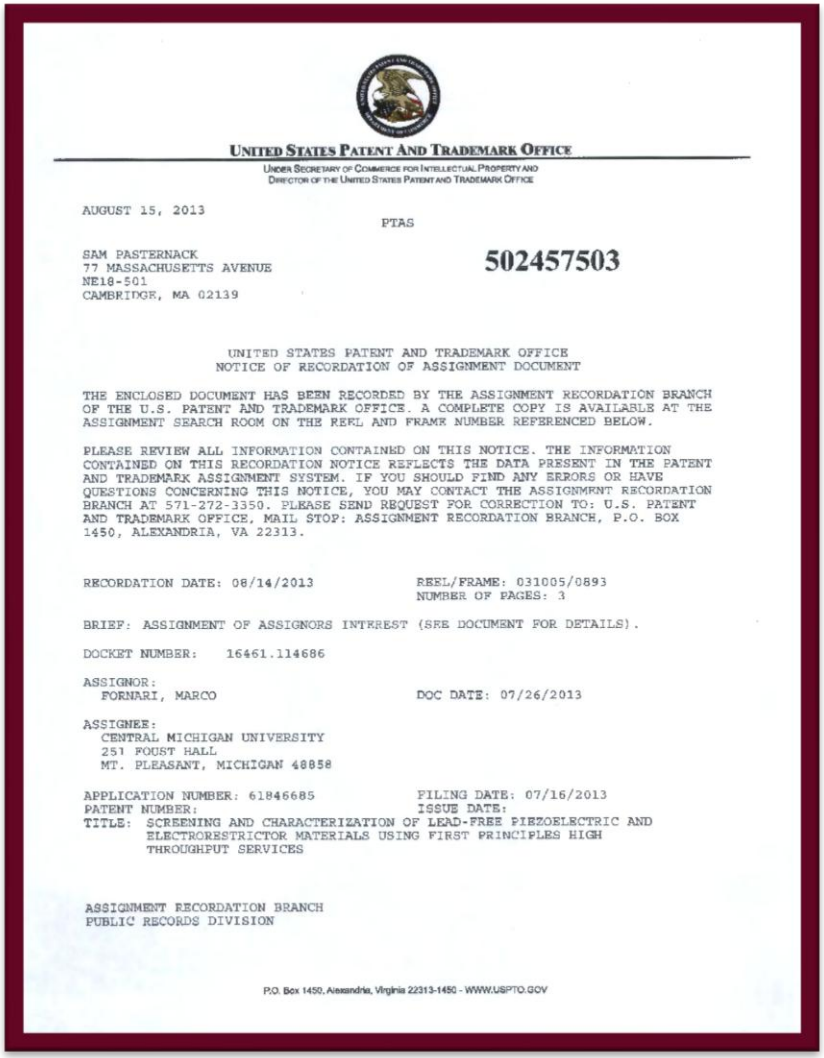




Descriptors application: piezoceramics

- 63^2 → C0: 99 → C1-3: 49
- Three main families:
  - $(Sn,Pb)(Zr,Ti,Hf)O_3$
  - $(Ba, Sr, Ca)(Zr,Ti,Hf)O_3$
  - $(Li,Na,K,Cs)(Nb,Ta)O_3$
- **Descriptors interpolation:**
  - $x\ E_1(V(x))+(1-x)\ E_2(V(x))$
- **Stability** vs. concentration
  - convex hull



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FILING DATE: 07/16/2013
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ISSUE DATE:
TITLE: SCREENING AND CHARACTERIZATION OF LEAD-FREE PIEZOELECTRIC AND ELECTRORESTRICTOR MATERIALS USING FIRST PRINCIPLES HIGH THROUGHPUT SERVICES

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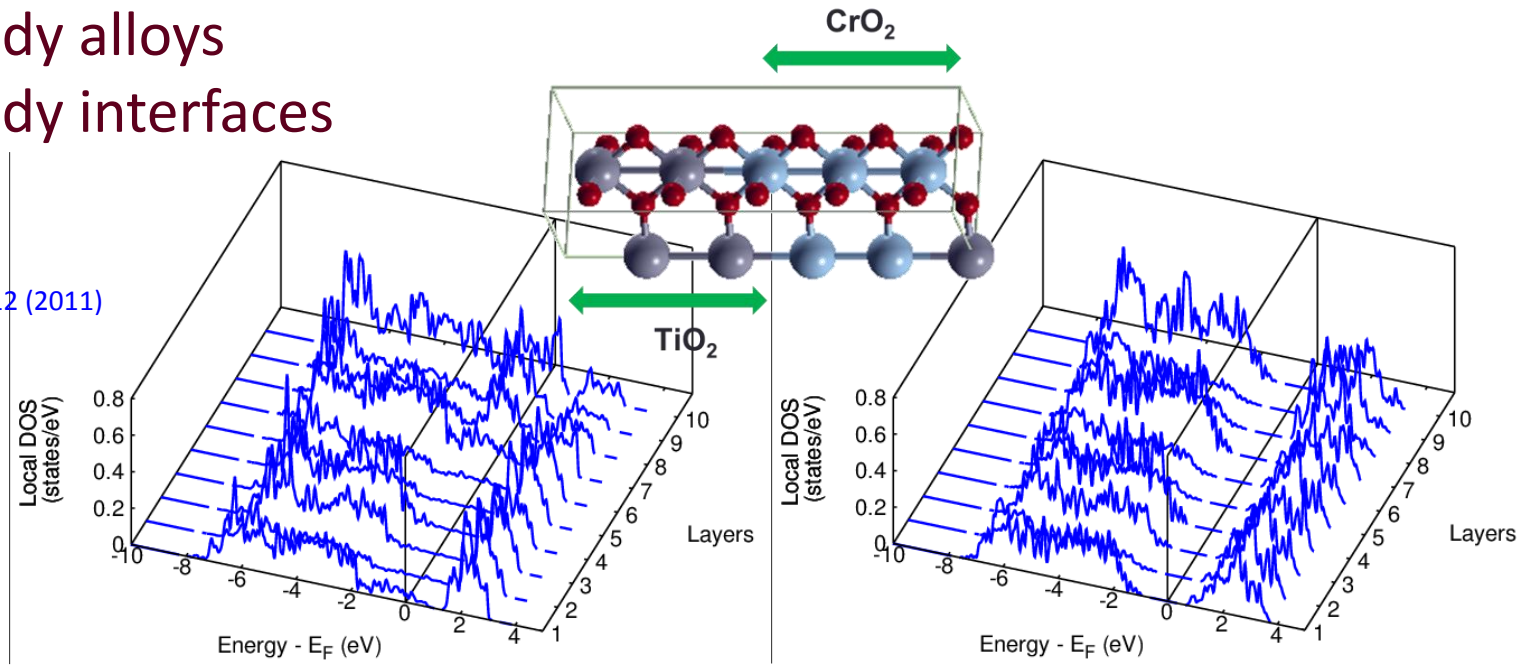
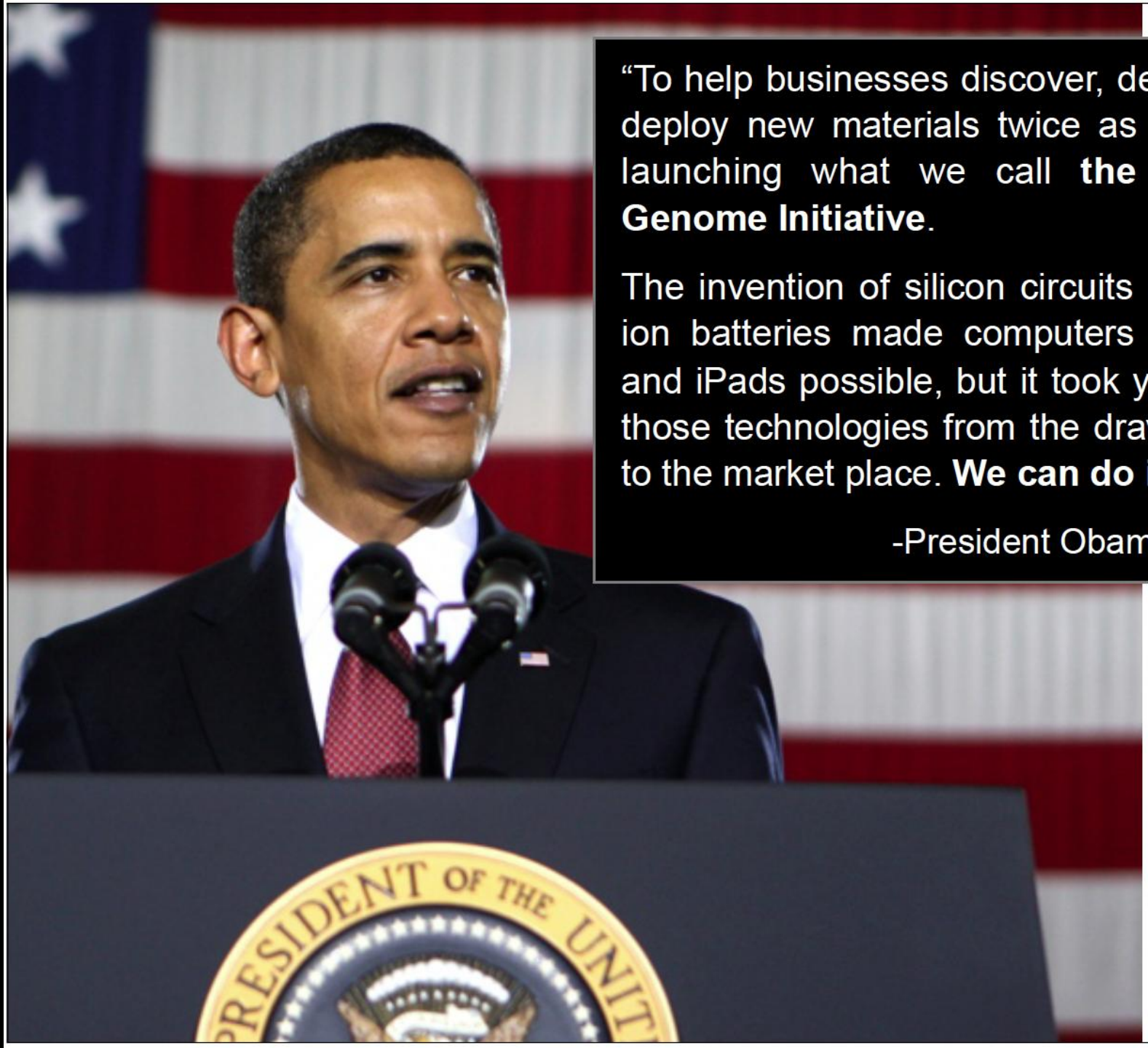
High-throughput calculations

- ✓ Accelerate the discovery of new chemical compositions/structures
- ✓ Study alloys
- ✓ Study interfaces

PRX **1**, 021012 (2011)



- ❖ Study nanostructuring effects … more to do
- ❖ Automatic search for descriptors … more to do
- ❖ Temperature dependent properties … more to do
- ❖ Morphological replacement … more to do
- ❖ Synthesis … more to do



"To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call **the Materials Genome Initiative**.

The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. **We can do it faster.**"

-President Obama (6/11)

Courtesy of Samsung Electronics

Fundamental Questions

- To which extent nano is real?
- Do we always need to think at structure-property relationships?
- What control is achievable in large scale nano manufacturing?
- What is the role of theory/calculations in nano manufacturing?

Fundamental Barriers

- Synergy between theory and … theory
- Synergy between theory and experiments
- Realistic goals that can be achieved
- Long term vs. short term research