Accelerated Materials Discovery

Turab Lookman

Los Alamos National Laboratory

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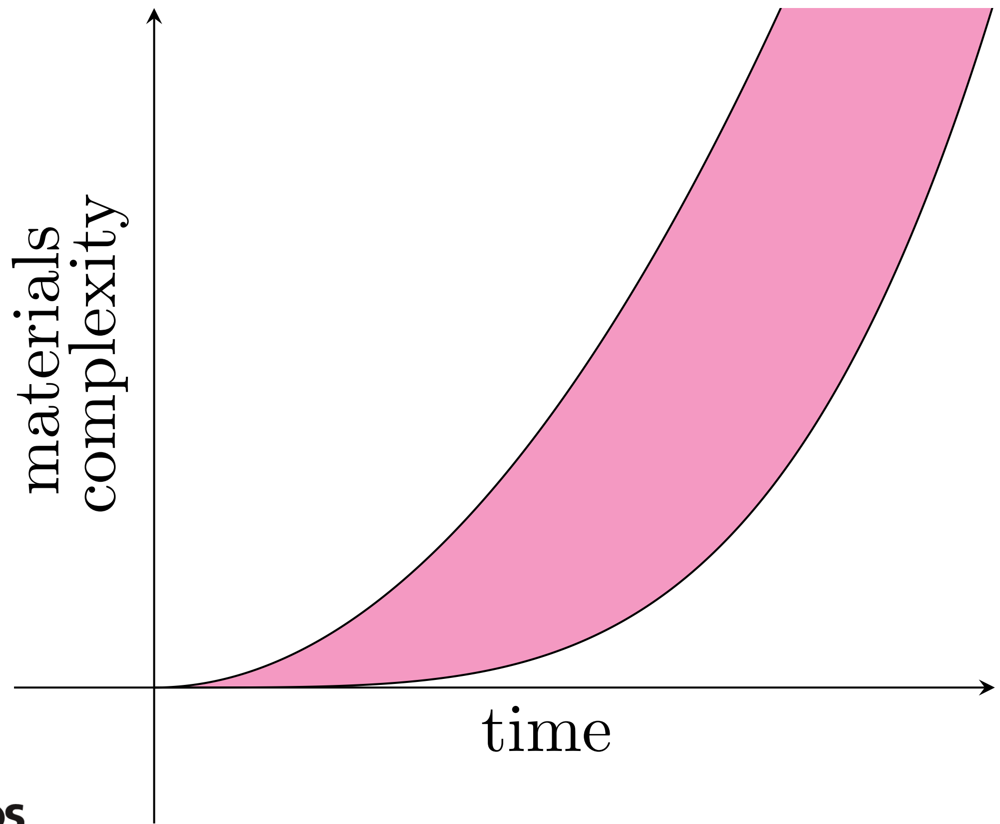
Q: How do we accelerate the process of selecting chemistry, composition, processing conditions to find materials with targeted properties ?



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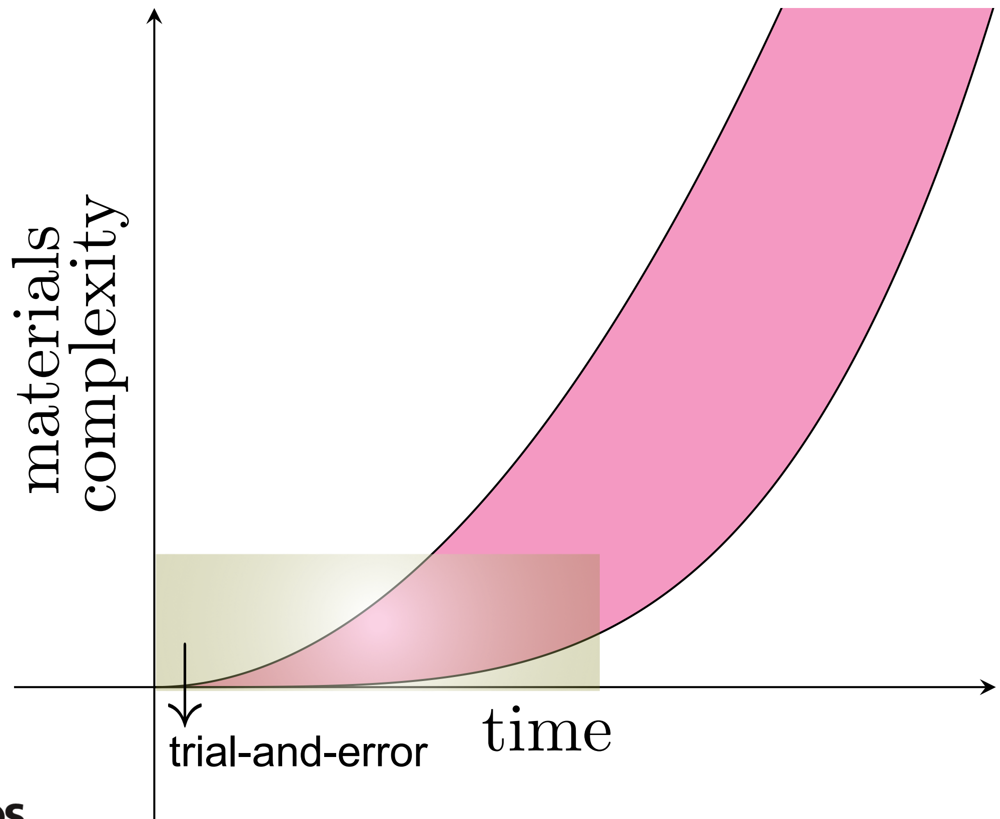

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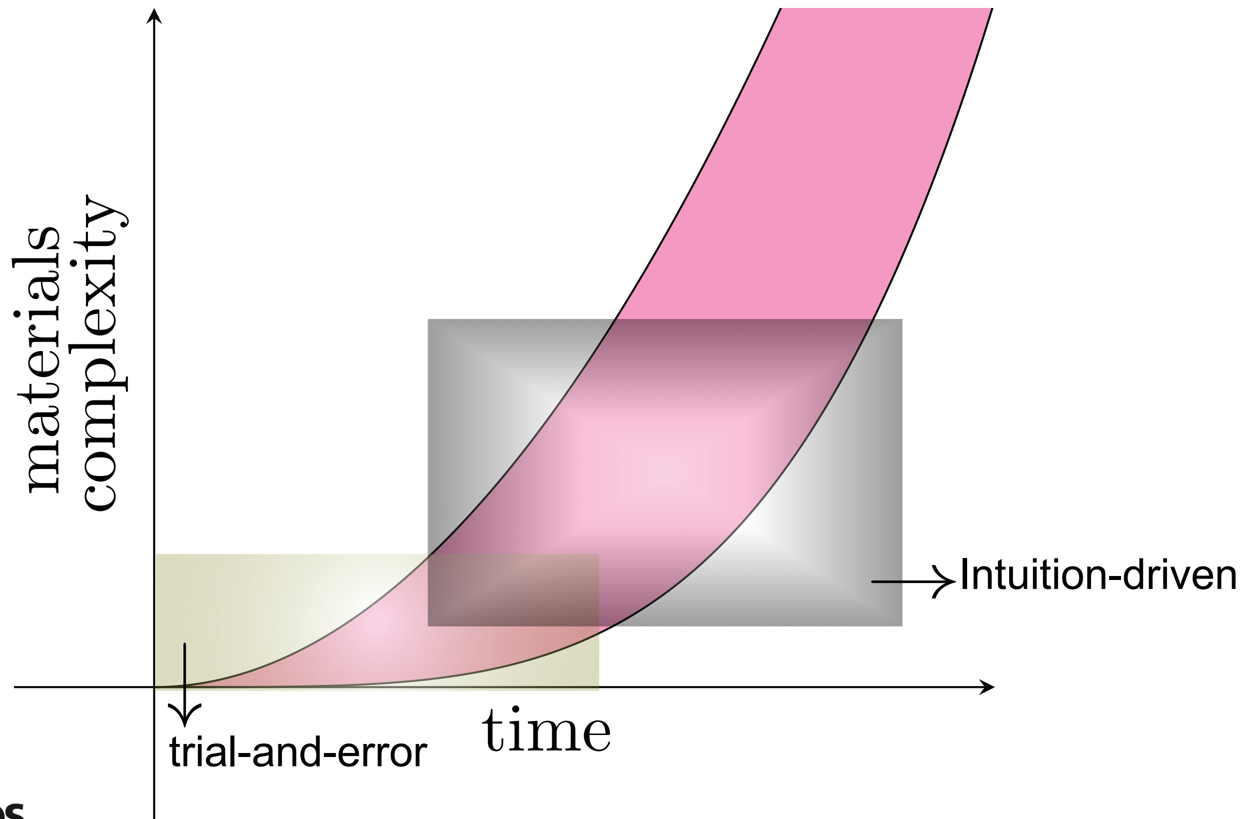

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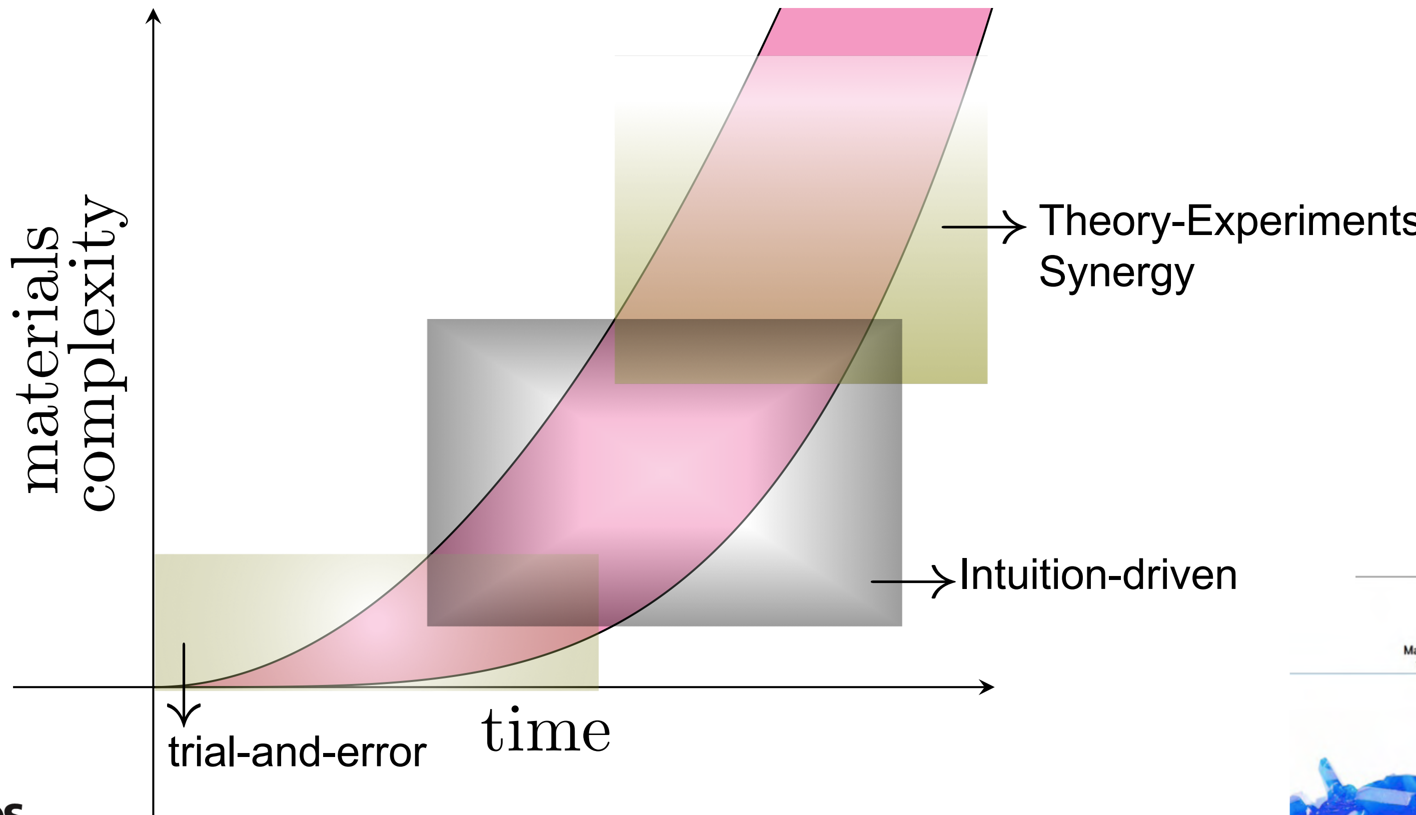

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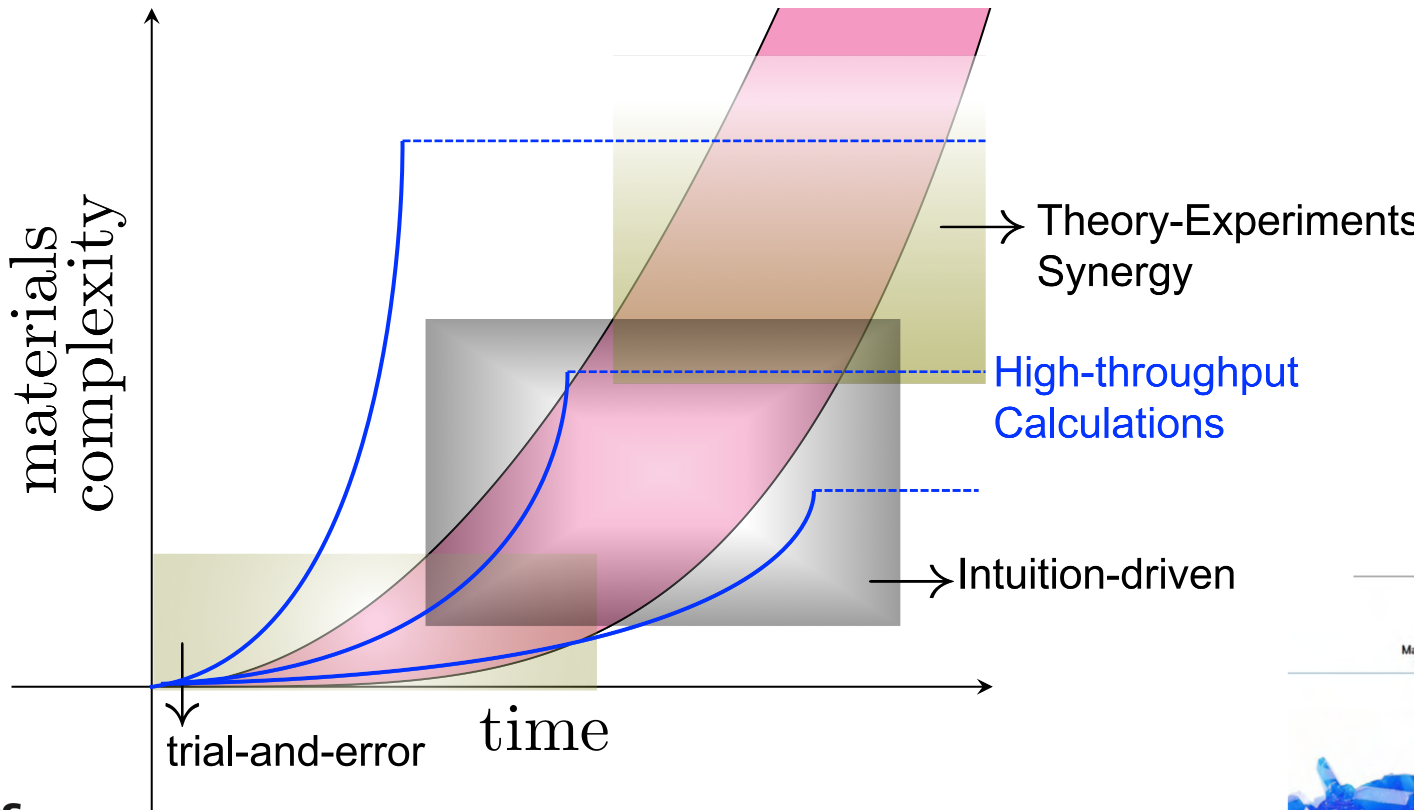

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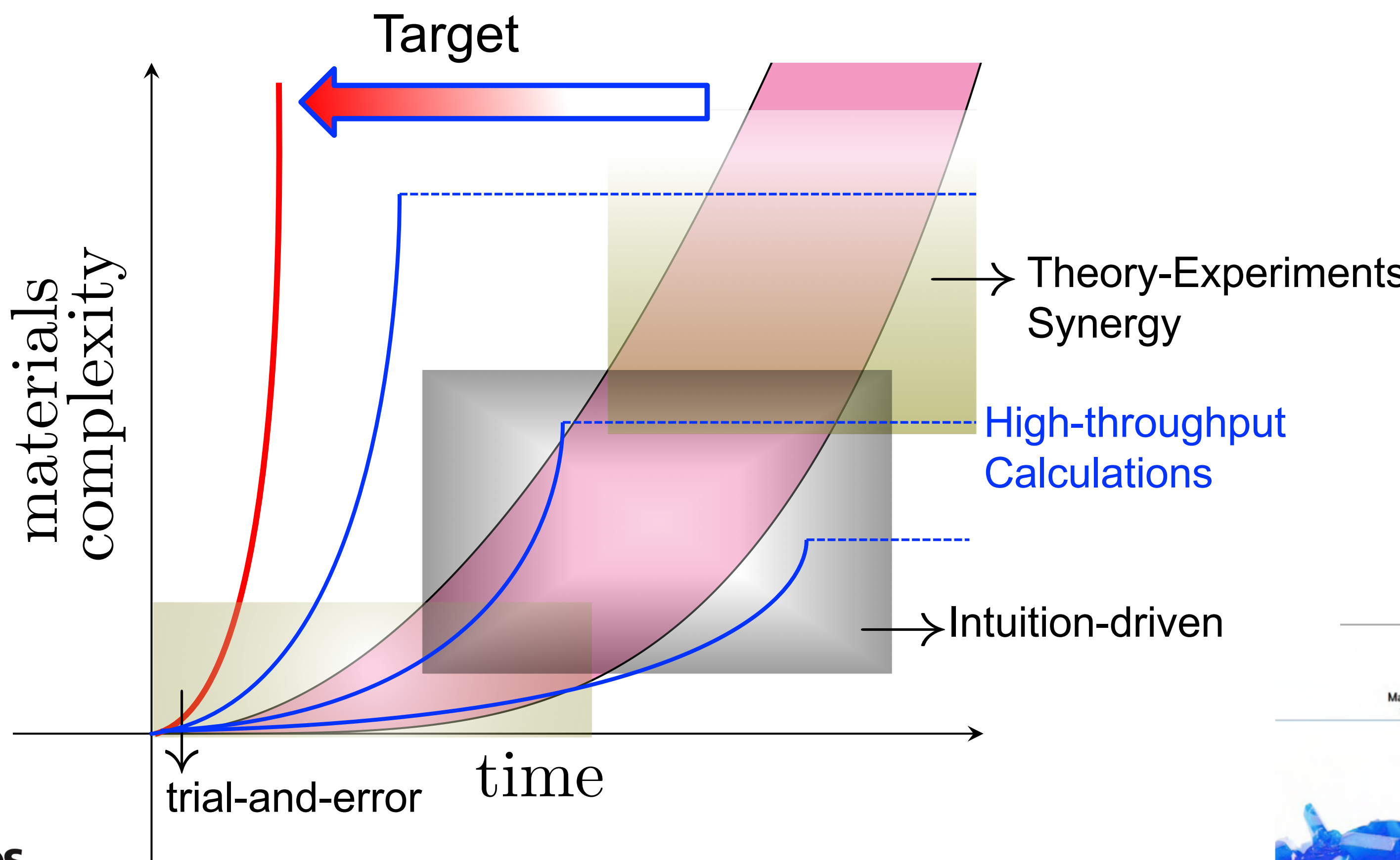
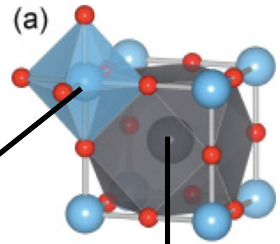


Materials discovery involves small amounts of data:

- Uncertainties, Multicomponent, vast search space
- **Search for better Pb-free piezoelectrics**

Computational Design

ABO_3



B

A

Screen for perovskite compounds

Chemical space of $63^2 = 3969$

99

Nonmetallic

$\Delta_{KS} > 0.25eV$

Small ΔE for distorted phases across MPB

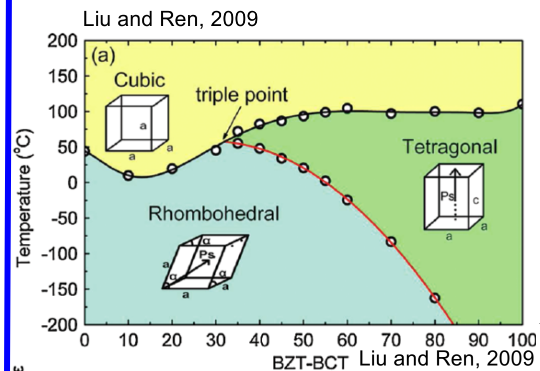
$\Delta E < 0.5eV$

49

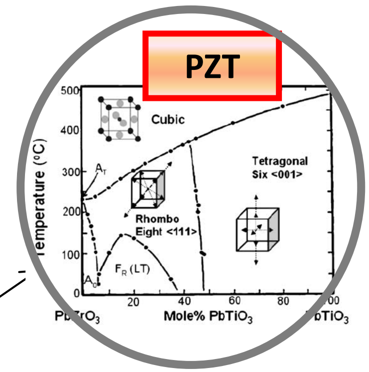
Armiento *et al. PRB* (2011)

Experimental Design

Liu and Ren, 2009



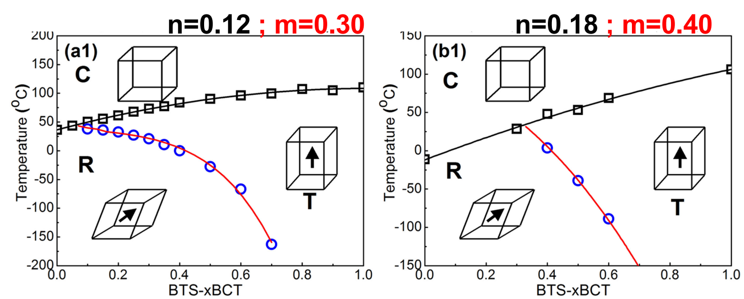
Liu and Ren, 2009



$Ba(Ti_{0.8}Zr_{0.2})O_3$

$(Ba_{0.7}Ca_{0.3})TiO_3$

$Ba(Ti_{1-m}X_m)O_3$-$x(Ba_{1-n}Y_n)TiO_3$



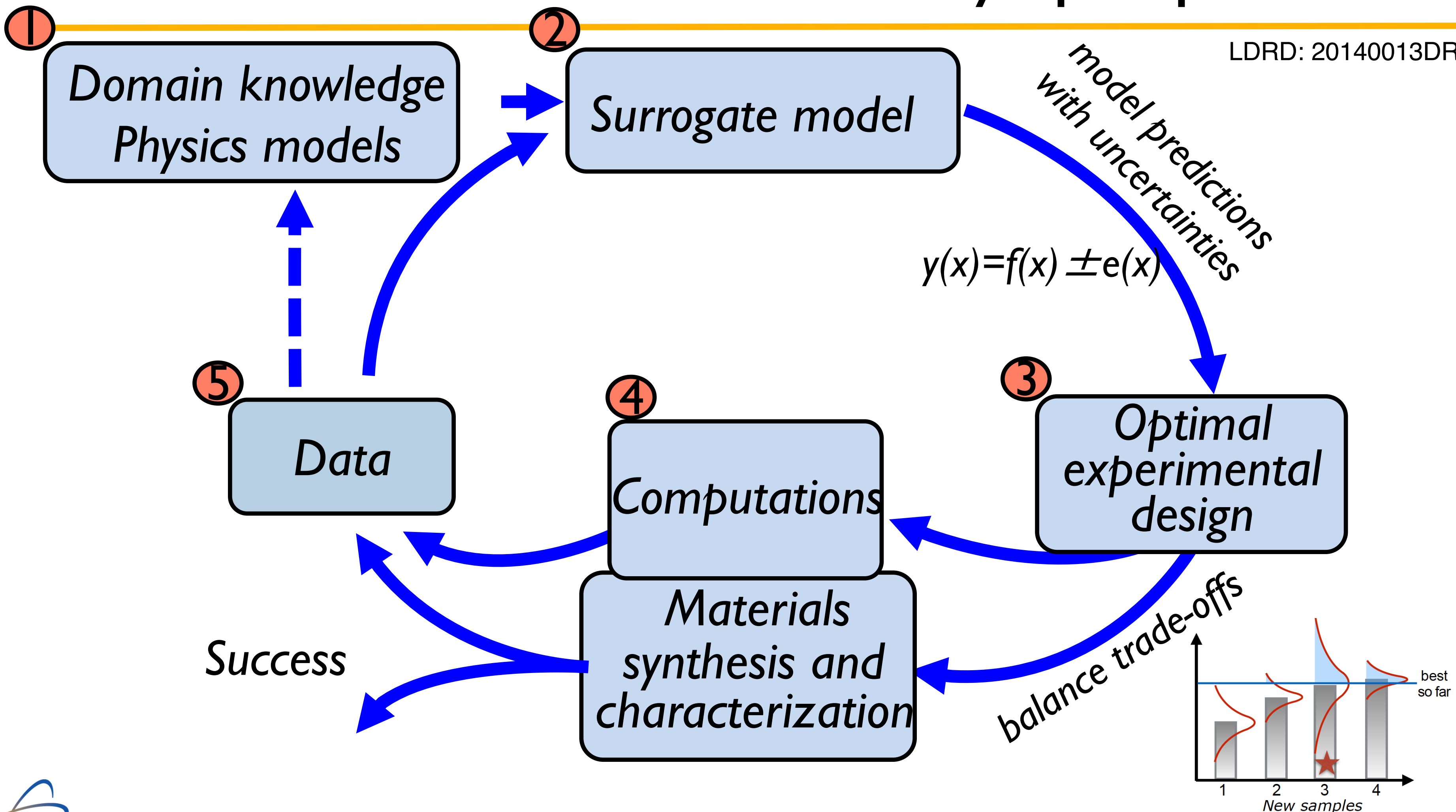
Xue et al, 2015

20 – 30 samples, search space ~ 10^3

Xue *et al. PNAS* (2016)

Adaptive Learning for materials discovery

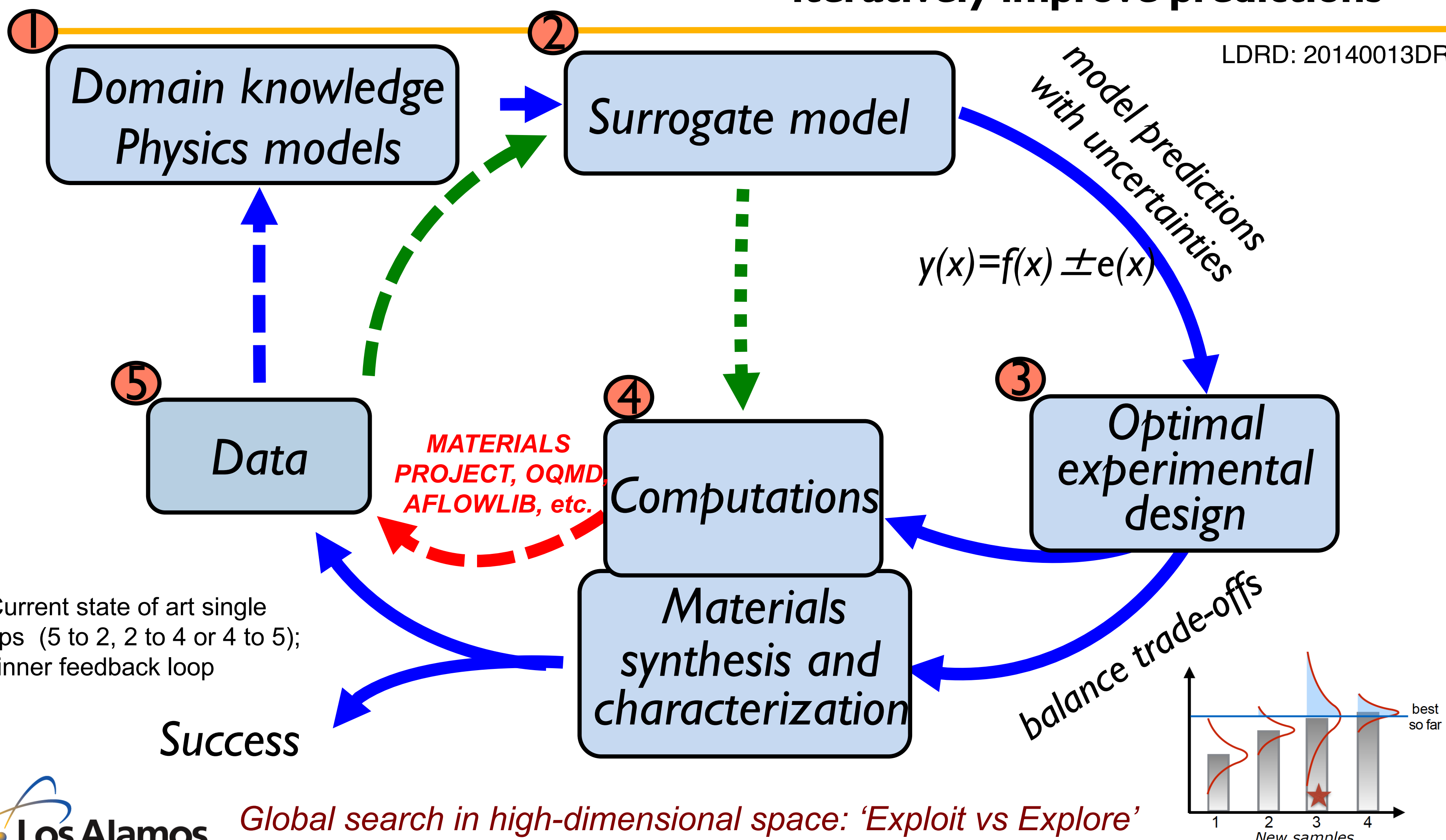
- **iteratively improve predictions**



Adaptive Learning for materials discovery

- **iteratively improve predictions**

LDRD: 20140013DR



Global search in high-dimensional space: 'Exploit vs Explore'

Bayesian Global Optimization large scale computational tasks OR experiments

Preliminary Experiments
Variables
Initial Designs

Response surfaces

Surrogate model

Bayesian

$\hat{y}$

New designs

Infill points

x

y

Function Evaluation

High fidelity, Expensive Computer Calculation

Value of Information (Howard' 65)
Utility functions (Lindley' 55,'72)

Bayesian Optimization

P[I] Kushner'64
E[I] Mockus'78
$E[I^g]$ Jones'88
Knowledge gradient (Powell)

Measurement Policies
Online: bandit problems
Offline :ranking and selection
: stochastic search

Probability Collectives
(Wolpert'98)

Constraints,
Multiobjective,
Multifidelity
Parallel function evaluations

Mean Objective Cost of Uncertainty (MOCU)
(Dougherty'2013)

T.L. *et al, Curr Opin in Sol Stat and Mat Sci.'* 2016

Design of Experiments (DOE)

Guide choice of experiments in an efficient manner

- **Factors X1, . . . Xk → Y**

- **Designs**
  Randomized Complete Block
  Factorial: Full, Fractional, Composite
  : Box-Behnken
  Random
  Latin HyperCube

Optimal Design : Find sample to optimize Y

$$y_i = f_\theta(x_i) \pm e_i$$

$$e \sim \mathcal{N}(0, \sigma)$$

$$y_i = \theta^T x_i \pm e_i$$

$$Var(\theta) = \sigma^2 (X^T X)^{-1} \qquad Var(y_i) = \sigma^2 \overbrace{(X^T X)}^{\mathbf{M_X}}{}^{-1} x_i$$

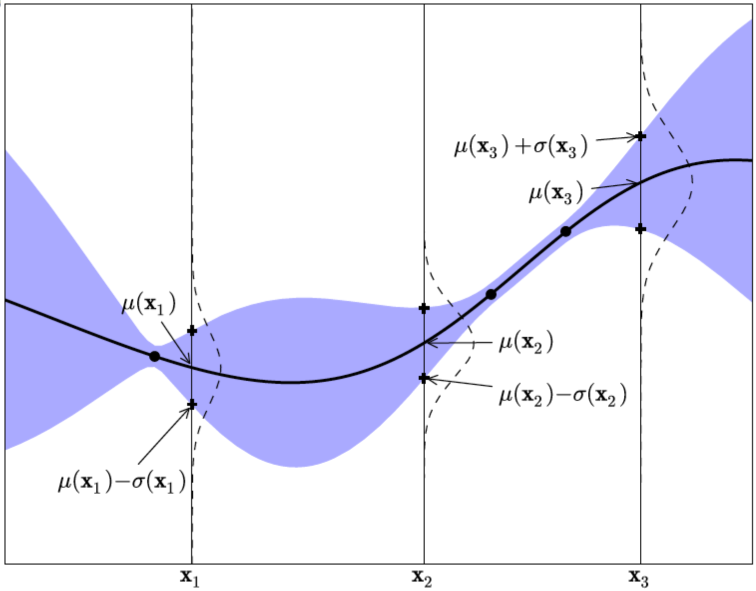
Optimal design	Objective
A-optimal	minimize trace $\{\mathbf{M}_X{}^{-1}\}$
D-optimal	minimize $\{\det \mathbf{M_X}\}^{-\frac{1}{p}}$
E-optimal	minimize max eigenvalue $\{\mathbf{M}_X{}^{-1}\}$
G-optimal	minimize max var $\{\mathbf{f}(\mathbf{x})\}$, $\mathbf{x} \in R$
I-optimal	minimize trace $\{\mathbf{MM_X}{}^{-1}\}$

Santner *et al.* ' 2003

Experimental design via Bayesian Optimization

$$\max_{\mathbf{x} \in \mathcal{A} \subset \mathbb{R}^d} f(\mathbf{x})$$

Step 1: Estimate objective $y_i = f(\mathbf{x}_i) + \varepsilon_i$



Data $\mathcal{D}_{1:t} = \{\mathbf{x}_{1:t}, f(\mathbf{x}_{1:t})\}$

$$\boxed{P(f|\mathcal{D}_{1:t}) \propto P(\mathcal{D}_{1:t}|f)P(f)}$$

Gaussian process $f(\mathbf{x}) \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}'))$

O'Hagan, 70

$$P(f_{t+1}|\mathcal{D}_{1:t}, \mathbf{x}_{t+1}) = \mathcal{N}\left(\mu_t(\mathbf{x}_{t+1}), \sigma_t^2(\mathbf{x}_{t+1})\right)$$

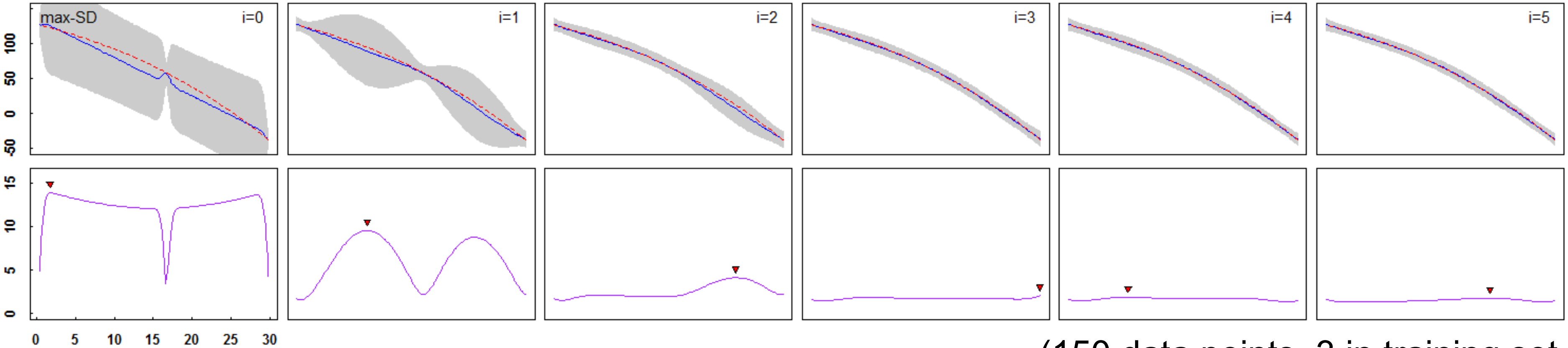
Posterior

Step 2: Sample with utility function

$$\mathbf{x}_t = \mathrm{argmax}_{\mathbf{x}}\, u(\mathbf{x}|\mathcal{D}_{1:t-1})$$

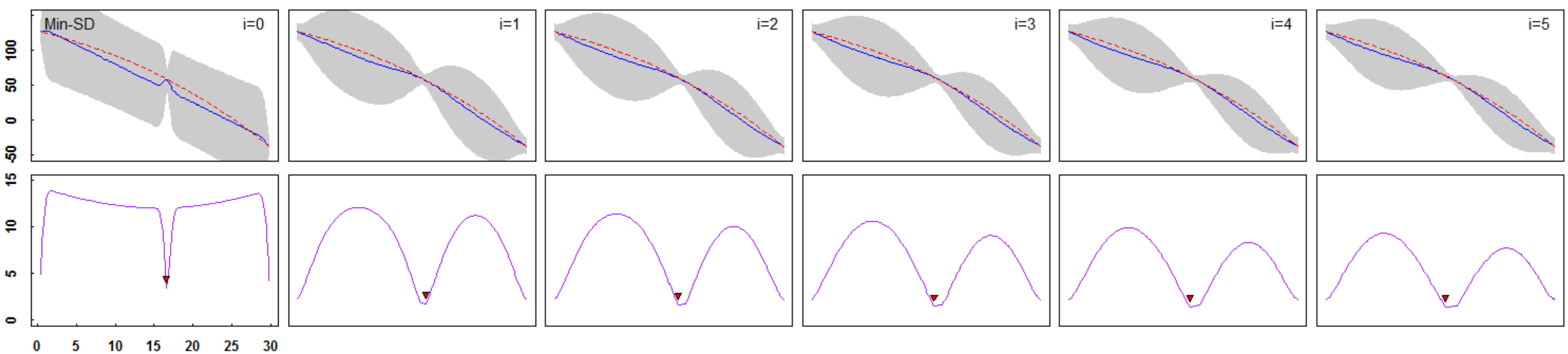
actual
predicted

Choose next point to ***maximize uncertainty****:*



(150 data points, 3 in training set.)

Choose next point to ***minimize uncertainty****:*

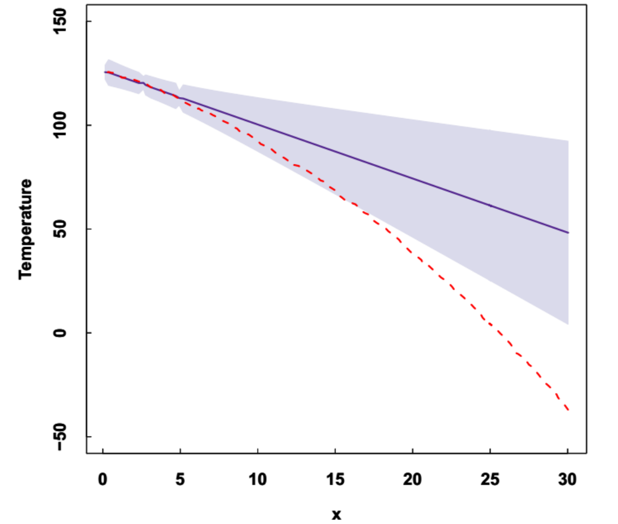


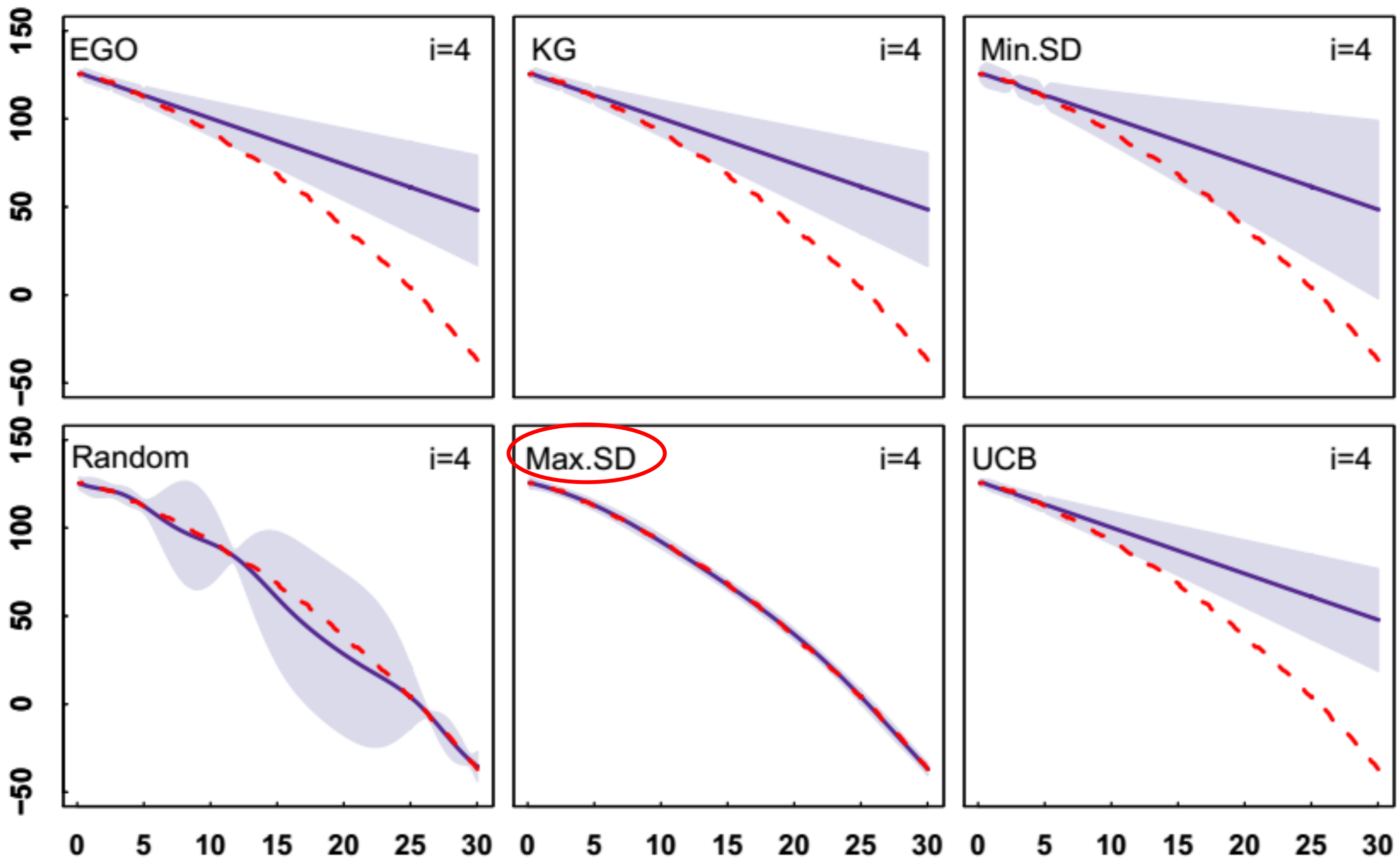
Utility functions: encoding decision criteria

- **Expected Improvement → EGO (Kushner, Mockus, Jones)**
- **Expected Quantile Improvement (Picheny)**
- **Lower or Upp. Confidence Bounds (Cox and Johnson, Srinivas)**
- **Sequential Kriging Optimization (Huang)**
- **Knowledge Gradient (Powell, Frazier)**
- **Mean Objective Cost of Uncertainty (Yoon, Xian, Dougherty)**
- **Maximum Variance**

Results

N_{train} = End 3

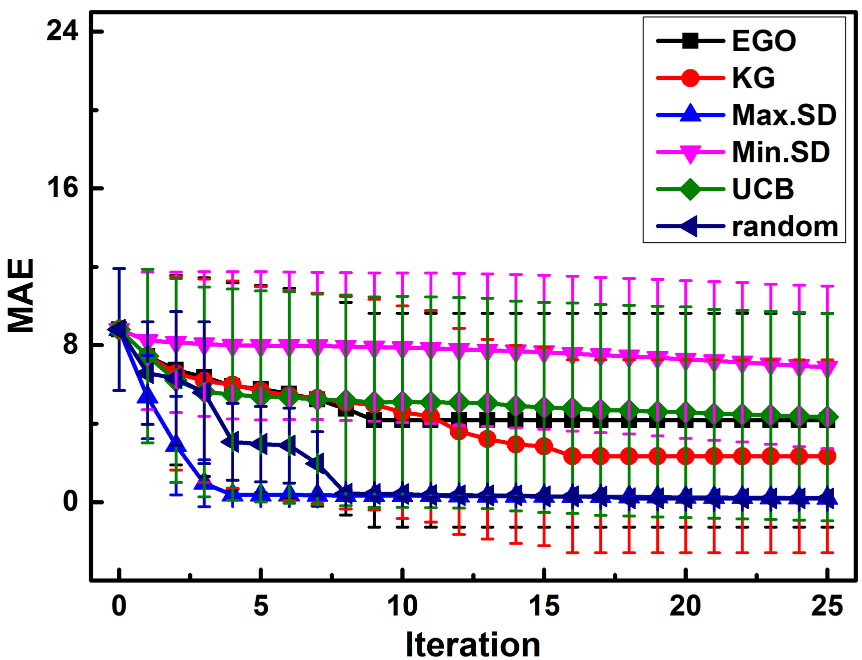


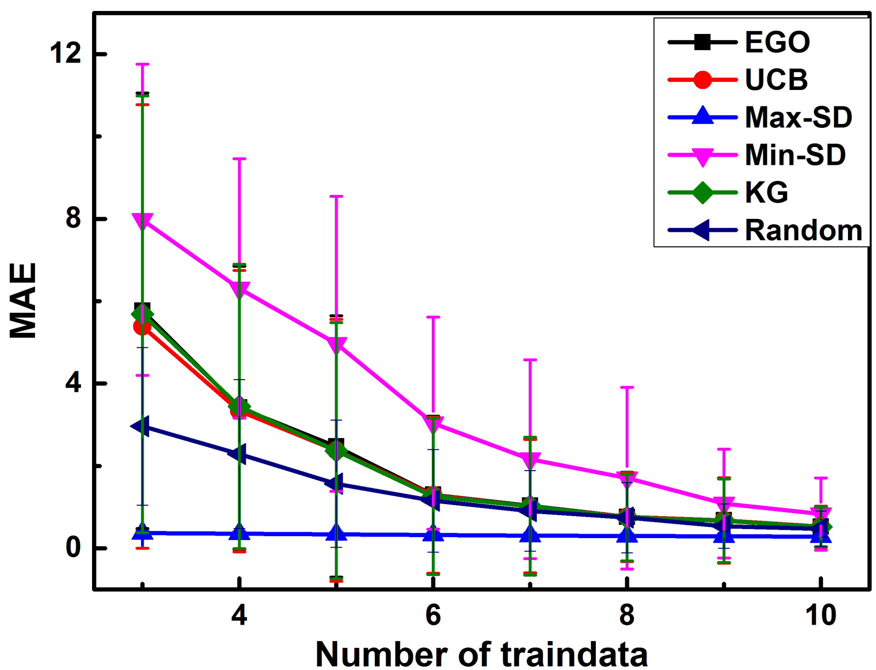


Results

N_{train} = sample 3

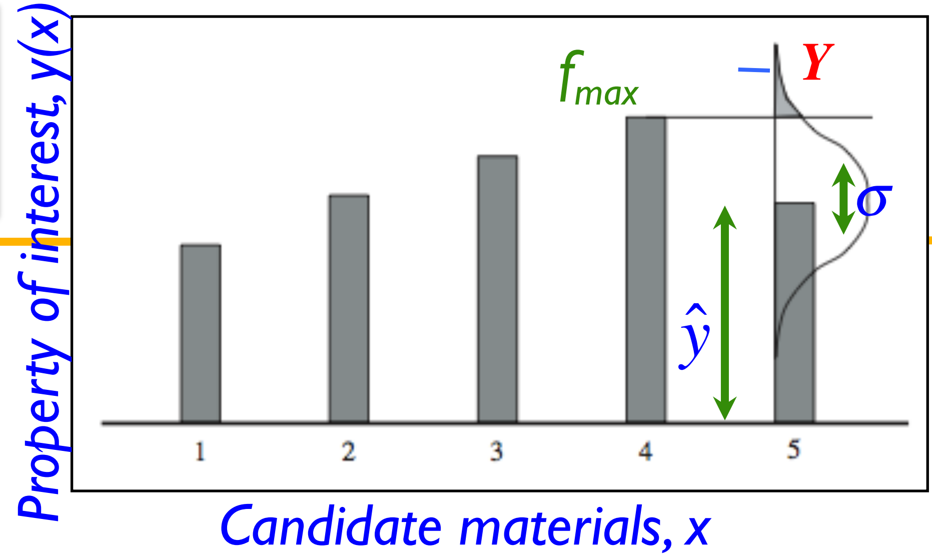
$$MAE = \frac{\sum_{i=1}^{n} |y_i - \mu|}{n}$$





Expected improvement

Mockus'78, Jones'88



Improvement: $I(x) = \max(Y - f_{max}, 0)$

$$E[I(x)] = \int_{f_{max}}^{\infty} (Y - f_{max}) P(Y \mid x') dY$$

$N(\hat{y}, \sigma^2)$

$$= (\hat{y} - f_{max})\Phi\left(\frac{\hat{y} - f_{max}}{\sigma}\right) + \sigma\phi\left(\frac{\hat{y} - f_{max}}{\sigma}\right)$$

Choose sample with largest "Expected Improvement": $x_i = \mathrm{argmax}_x\,[E(I(x))]$

Limiting cases:

Small σ $\quad E \rightarrow \hat{y} - f_{max}$

Choose $\hat{y}$ better than best-so-far f_{max}

Exploitation *(local, utilize model)*

Large σ $\quad E \rightarrow \sigma$

Choose $\hat{y}$ with largest uncertainty σ

Exploration *(global, improve model)*

Mean Objective Cost of Uncertainty

Identify experiment expected to maximally reduce MOCU one step ahead

Assume cost function, $g(\theta; c)$

θ Unknown parameters
c characterizes an experiment
e.g. material composition

If θ known, then the optimal material would be $c'_\theta = \arg\min_{c \in C} \mathrm{g}(\theta; c)$

If θ unknown, then the robust material is $c'' = \arg\min_{c \in C} \mathrm{E}_\theta[\mathrm{g}(\theta; c)]$

Expected Loss in using robust instead of optimal

$$MOCU = \mathrm{E}_\theta[\underbrace{g(\theta; c'_\theta)}_{\text{Property of optimal material at state } \theta} - \underbrace{g(\theta; c'')}_{\text{Property of IBR material across all } \theta}]$$

Dehghannasiri, R., Yoon, B-J., and E. R. Dougherty, "**Optimal Experimental Design for Gene Regulatory Networks in the Presence of Uncertainty**," *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, 2016

MOCU: Selection of next experiment

- Experiments $C1, C2, C3, etc$ Outcomes: c_1, c_2, c_3

Remaining after outcome c_i $MOCU = \mathrm{E}_{\theta|Ci=c_i}[g(\theta;c'') - g(\theta;c'_\theta)]$

Conditional distribution $f(\theta|Ci = c_i)$

Using Bayes, obtain $f(c|\theta)$

Expected remaining MOCU given that experiment c_i undertaken:

$$MOCU_i = \mathrm{E}_{c_i}\mathrm{E}_{\theta|Ci=c_i}[g(\theta;c'') - g(\theta;c'_\theta)]$$

$$c_i^* = \arg\min_{i \in 1,..n} MOCU_i$$

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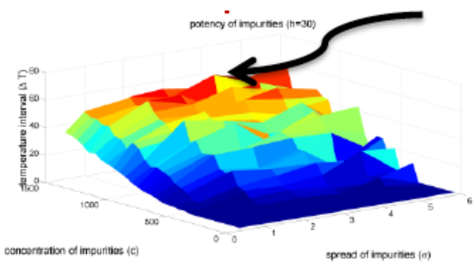
journal homepage: www.elsevier.com/locate/commatsci

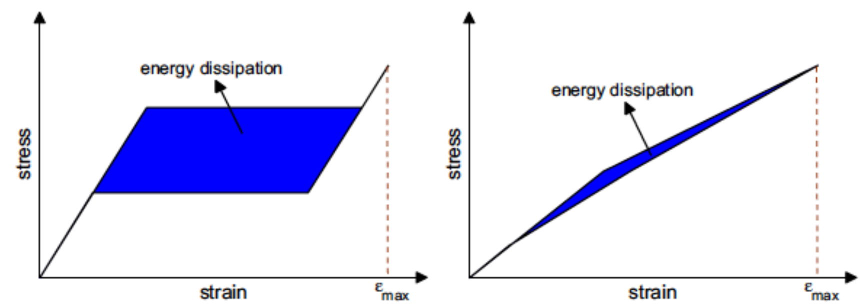
Optimal experimental design for materials discovery

Roozbeh Dehghannasiri [a,b,*], Dezhen Xue [c,d], Prasanna V. Balachandran [c], Mohammadmahdi R. Yousefi [e], Lori A. Dalton [e,f], Turab Lookman [c,*], Edward R. Dougherty [a,b,*]

Problem: Minimize energy dissipation by selecting optimal dopants in as few experiments as possible



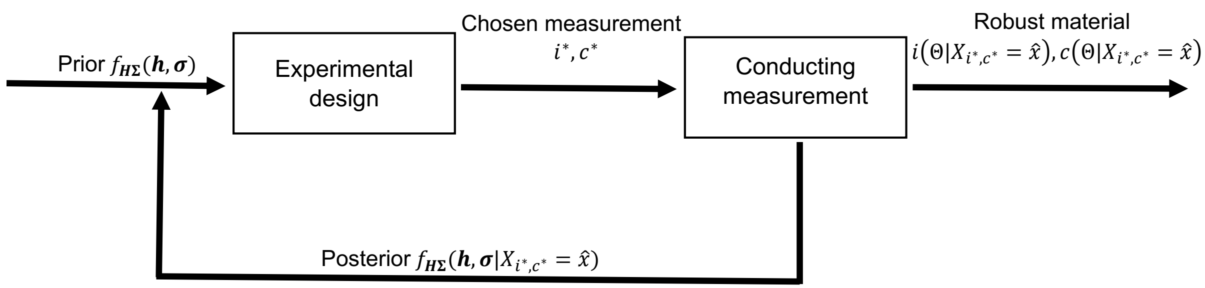
$$\rho(\vec{r}) = h\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{\vec{r}^2}{2\sigma^2}}.$$

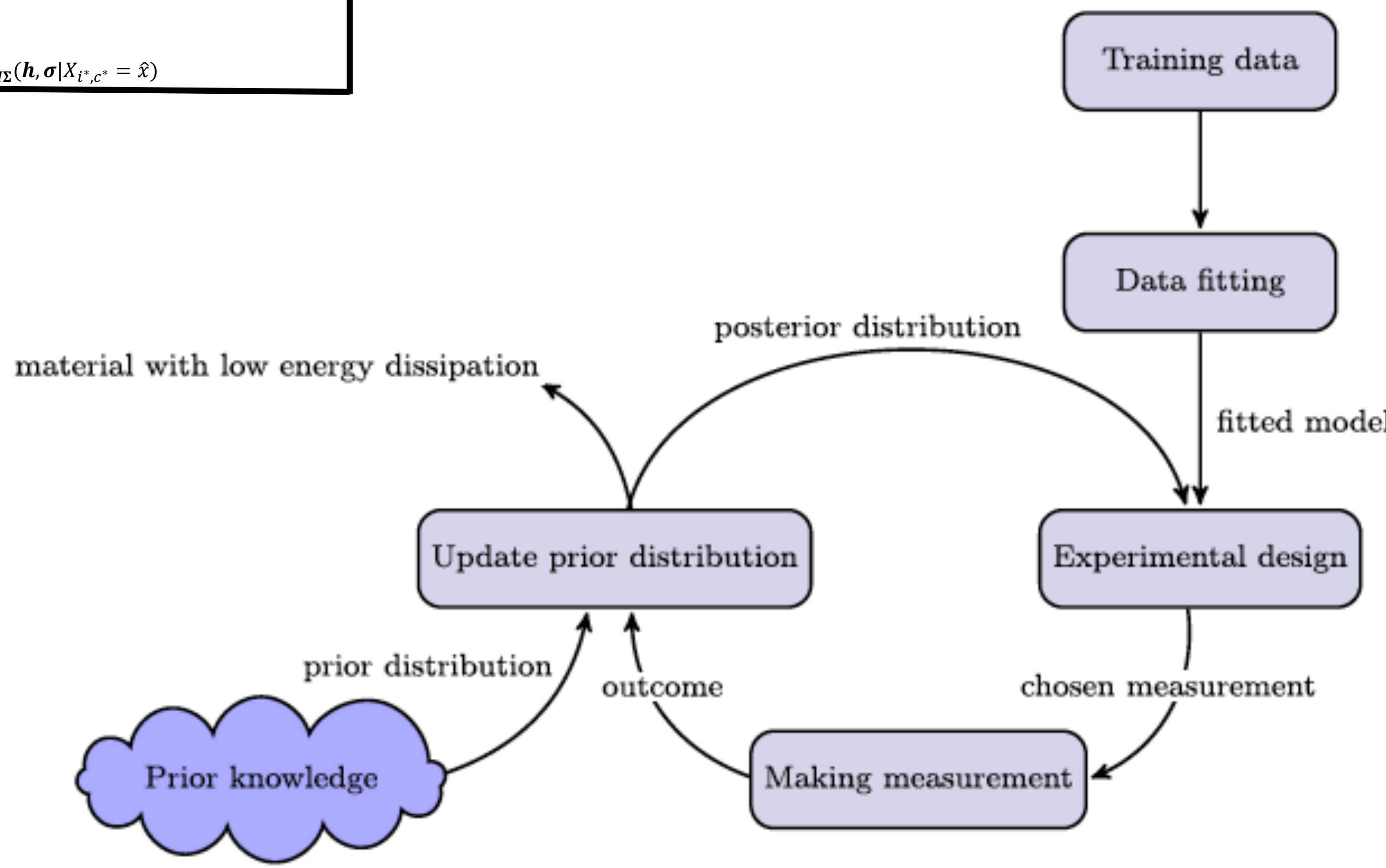


Use physics based model as surrogate for objective:

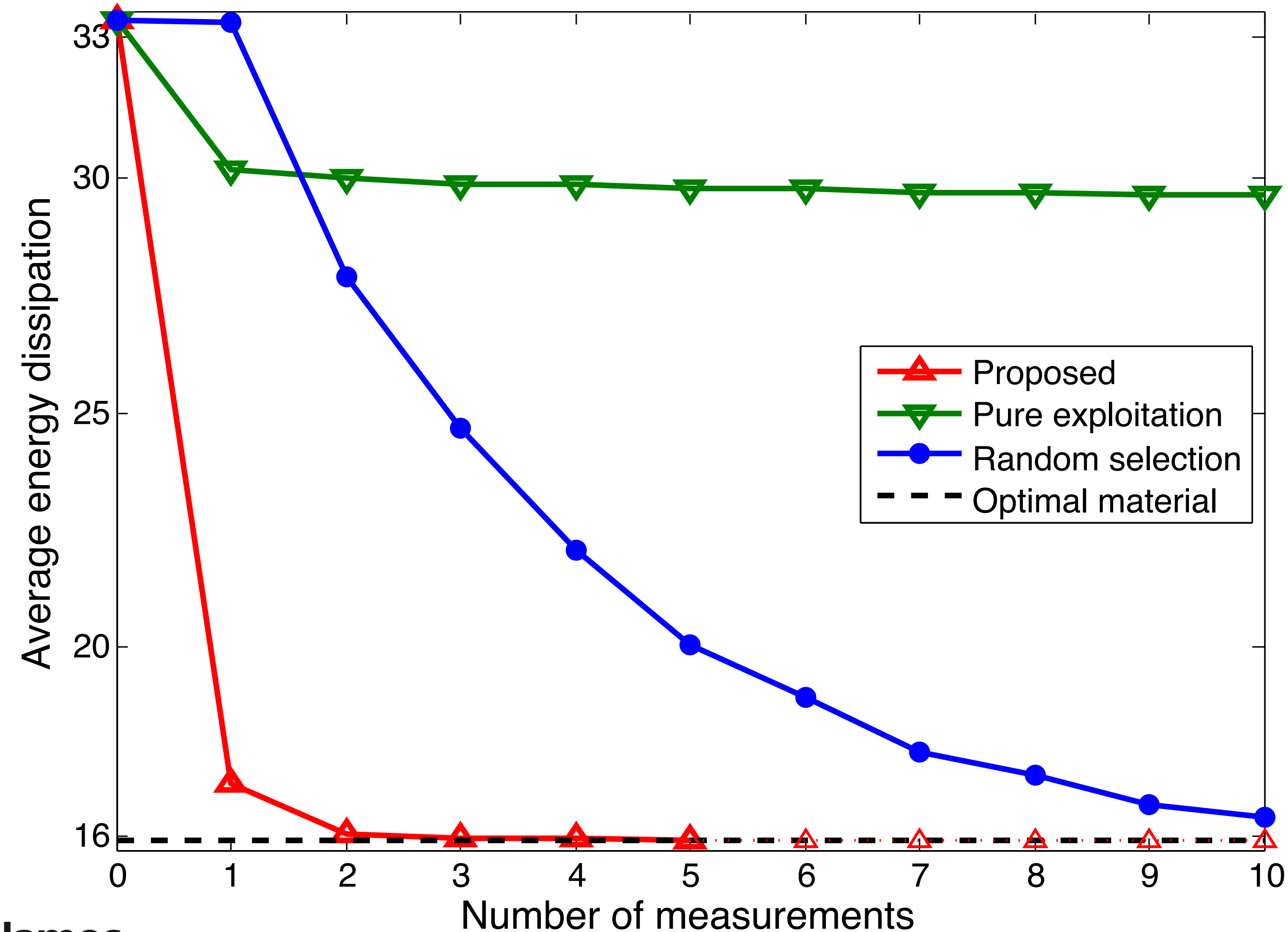
$$g(h,\sigma,c;\mathbf{b}) = \max\left(\frac{1}{(b_1 h + b_2\sigma + b_3 h\sigma + b_4)c + b_5 h + b_6\sigma + b_7 h\sigma + b_8}, 0\right),$$

Active learning loop

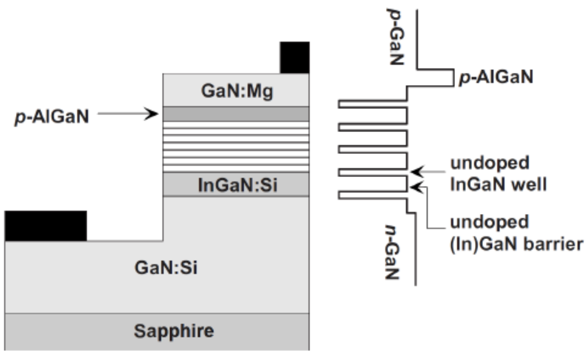




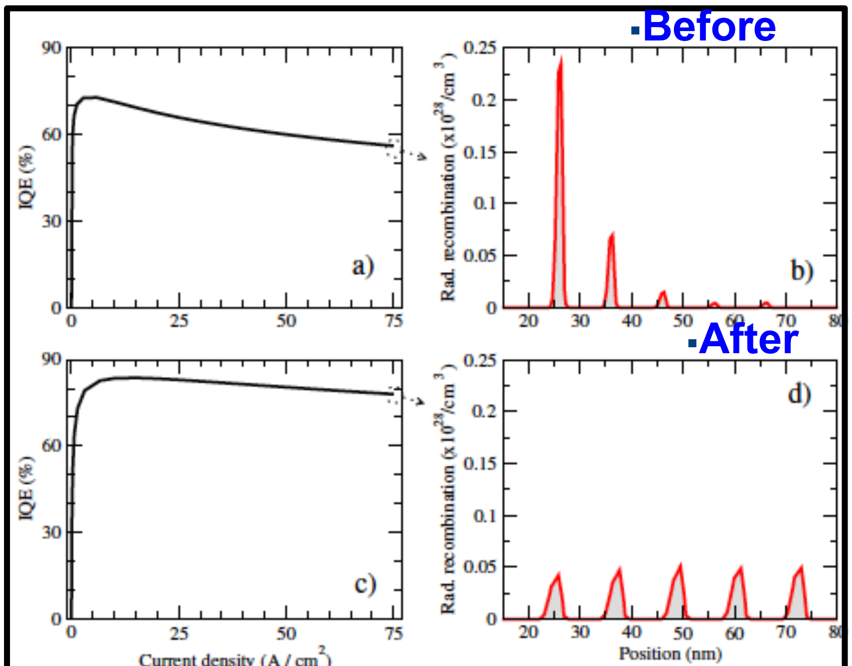
Comparison with several strategies

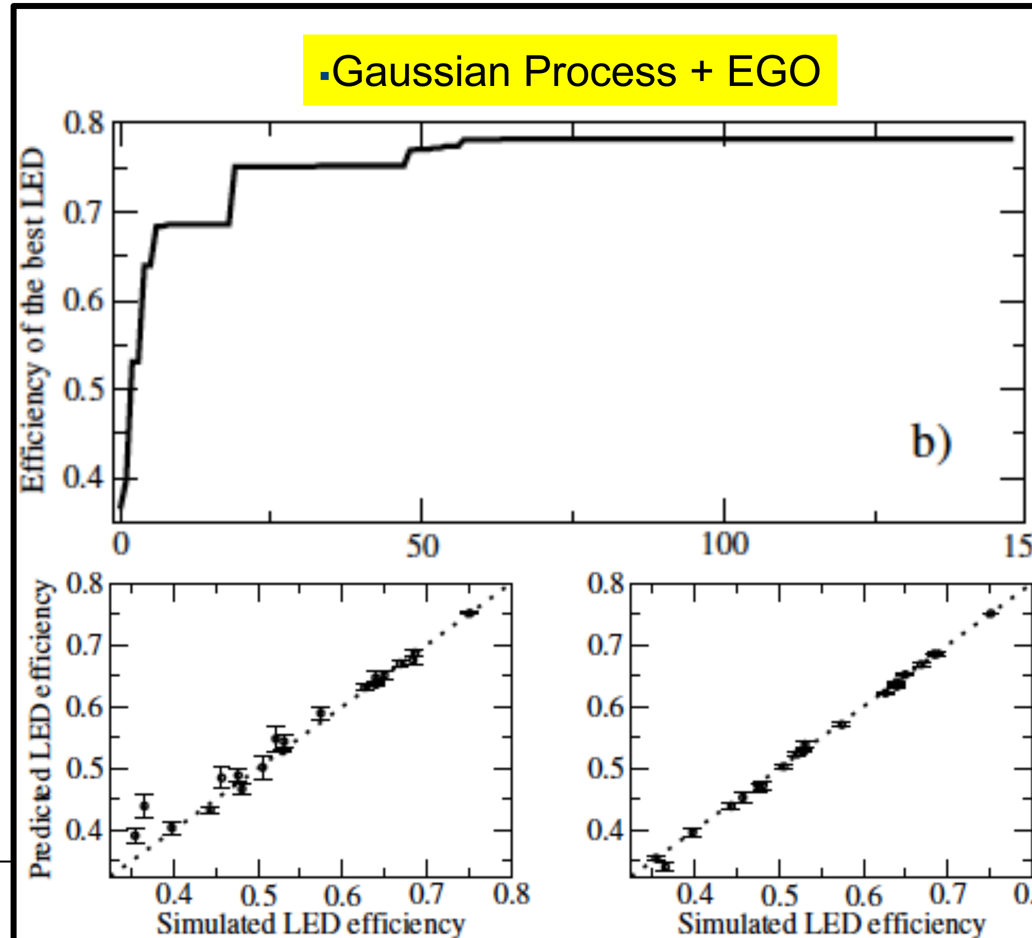


Optimize codes: LED structures for highest efficiencies at high currents



Quantum Efficiencies ← APSYS code ← Features: barrier height 5 quantum wells



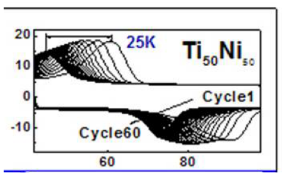


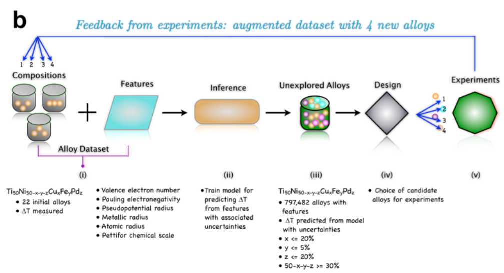
Leduc *et al.*, 2016

Examples

Data-driven ⟷ *Experiments* ⟷ *Use theory with data* ⟷ *Experiments*

Strategy: $Ti_{50}\ Ni_{50\text{-}x\text{-}y\text{-}z}\ Cu_x\ Pd_y\ Fe_z$
Total possibilities: 800,000 (22 known)
Target: Minimize Thermal Hysteresis





36 experiments
14 with superior properties

Xue *et al.*, Nature Comm., 2016

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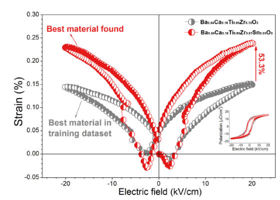
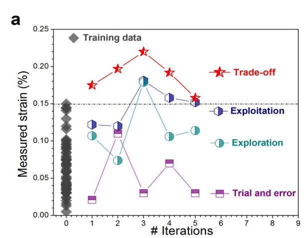
Materials Discovery — www.advmat.de

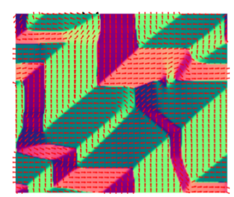
Accelerated Discovery of Large Electrostrains in $BaTiO_3$-Based Piezoelectrics Using Active Learning

$$(Ba_{100-x-y}Ca_xSr_y)(Ti_{100-u-v}Zr_uSn_v)O_3$$

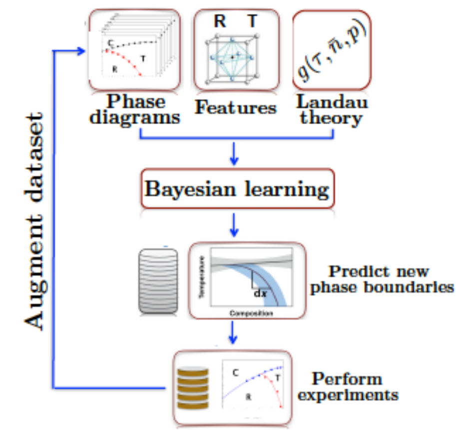
- Largest electrostrain

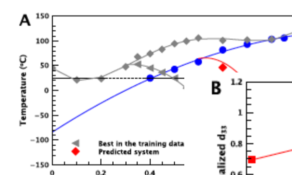


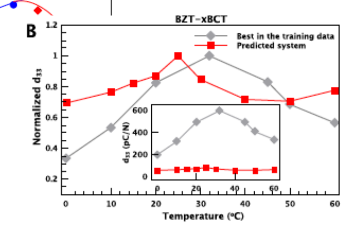




Yuan *et al.*, Advanced Materials, 1702884 2018







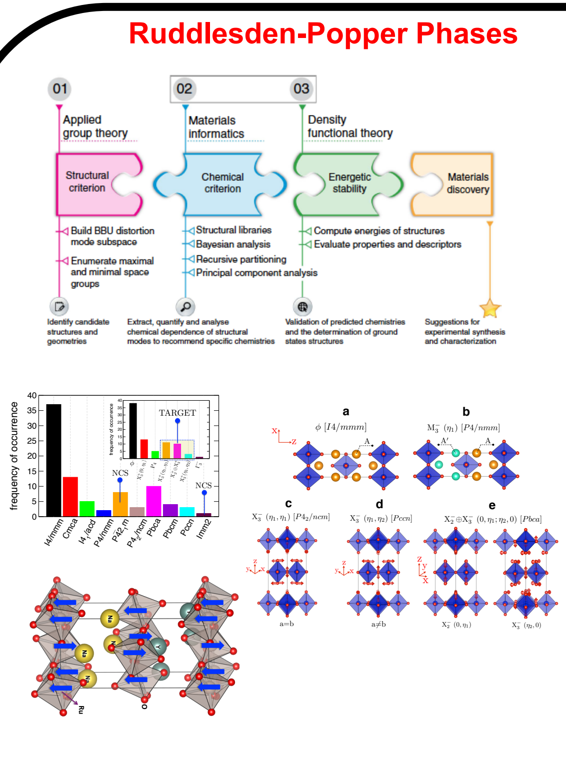
Xue *et al.*, PNAS, 2016

Computations

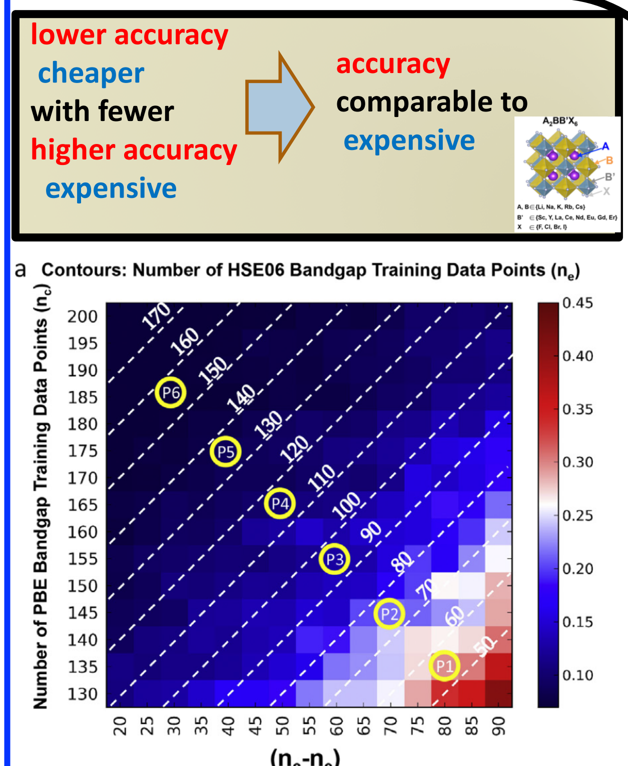
Predict new materials

Multi- fidelity data

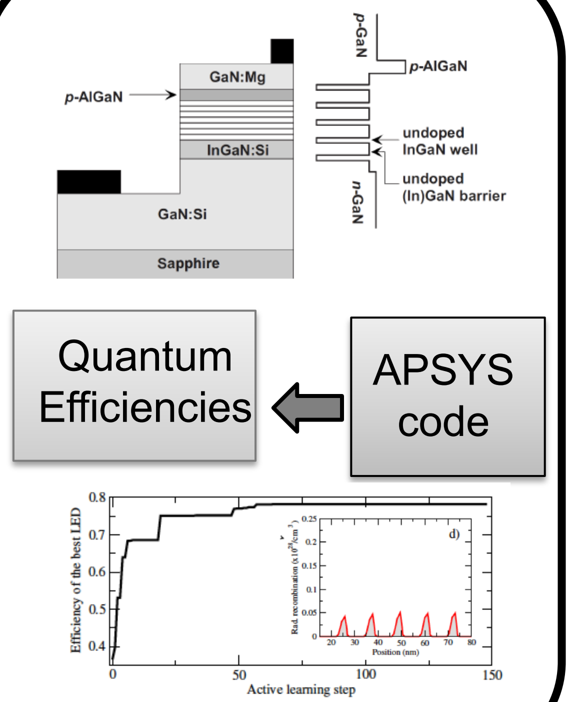
Accelerate codes



Balachandran *et al.*, Nature Comm., 2017

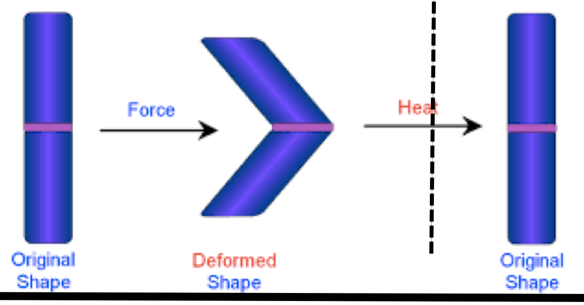


Pilania *et al.*, Computational Materials Sci, 2017

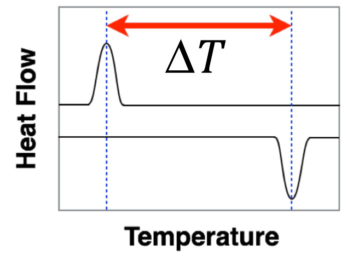


Leduc *et al.*, Sci. Rep, 2016, APL 2017

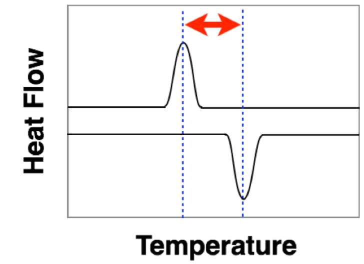
Example: Find NiTi alloy with lowest hysteresis

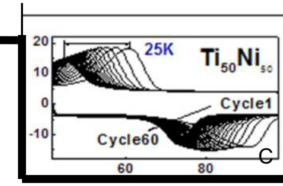


Thermal hysteresis



Desire





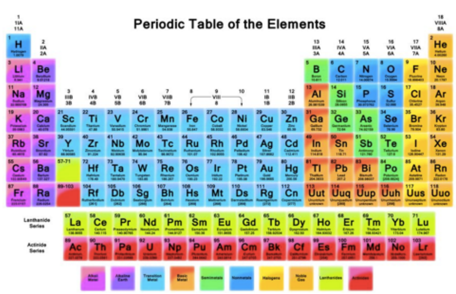
Strategy: $Ti_{50}\ Ni_{50\text{-}x\text{-}y\text{-}z}\ Cu_x\ Pd_y\ Fe_z$

Search space of multicomponent alloy ~800K
22 training samples (.003%) with measured ΔT

$$x \le 20\%, y \le 5\%, z \le 20\%$$

$$50 - x - y - z \ge 30\%$$

Composition control 0.1%



Knowledge:

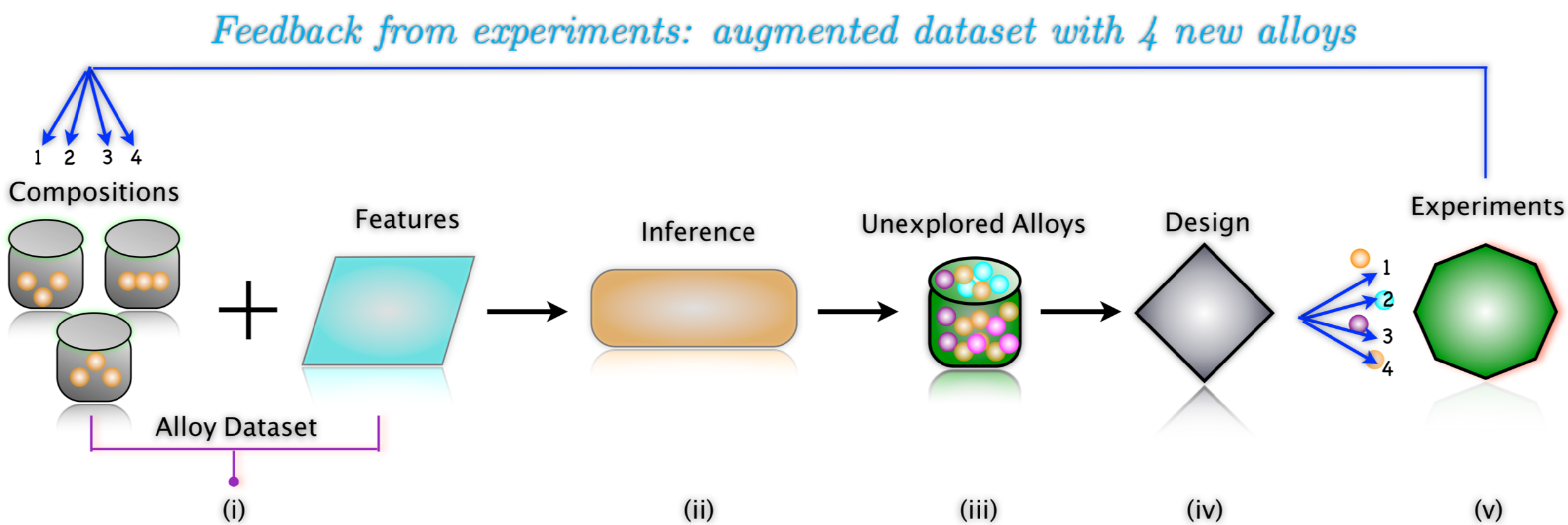
- **Transition temperatures influenced by valence electron concentration**
- **Hysteresis influenced by atomic size**
- **Relative stability influenced by changes in electron number**

Features:

Valence electron number
Radii: metallic, Clementi, Zunger
Electronegativity
Pettifor Chemical scale

Each $Ti_{50}\ Ni_{50\text{-}x\text{-}y\text{-}z}\ Cu_x\ Pd_y\ Fe_z$ weighted fraction of features

Adaptive Design for Alloy Discovery



(i)

$Ti_{50}Ni_{50-x-y-z}Cu_xFe_yPd_z$

- 22 initial alloys
- ΔT measured

- Valence electron number
- Pauling electronegativity
- Pseudopotential radius
- Metallic radius
- Atomic radius
- Pettifor chemical scale

(ii)

- Train model for predicting ΔT from features with associated uncertainties

(iii)

$Ti_{50}Ni_{50-x-y-z}Cu_xFe_yPd_z$

- 797,482 alloys with features
- ΔT predicted from model with uncertainties
- x <= 20%
- y <= 5%
- z <= 20%
- 50-x-y-z >= 30%

(iv)

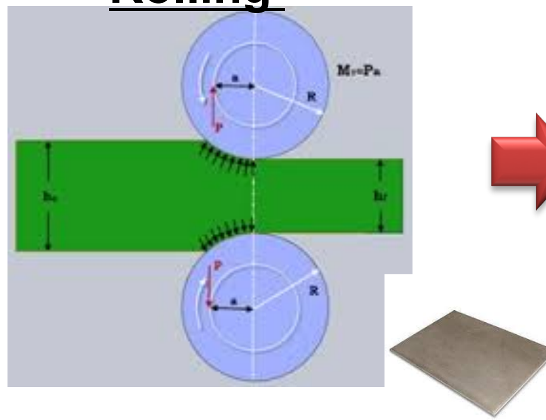
- Choice of candidate alloys for experiments

Xue *et al.*, Nature Comm., 2016

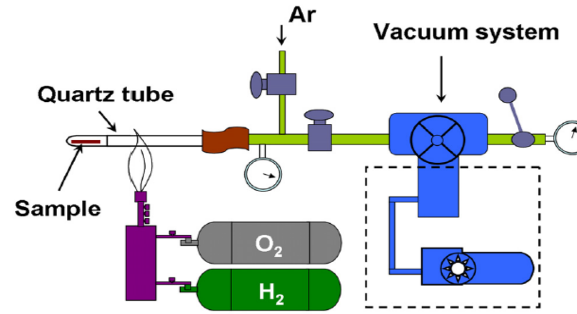
Experiments

Melting

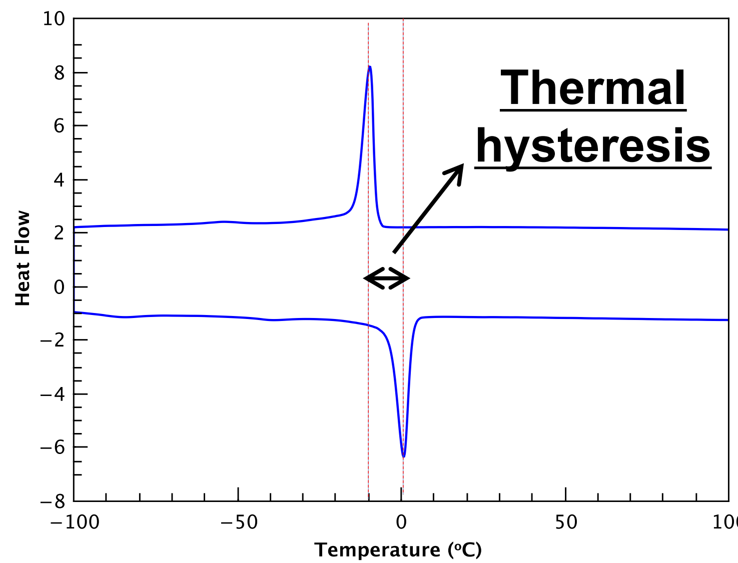
Rolling



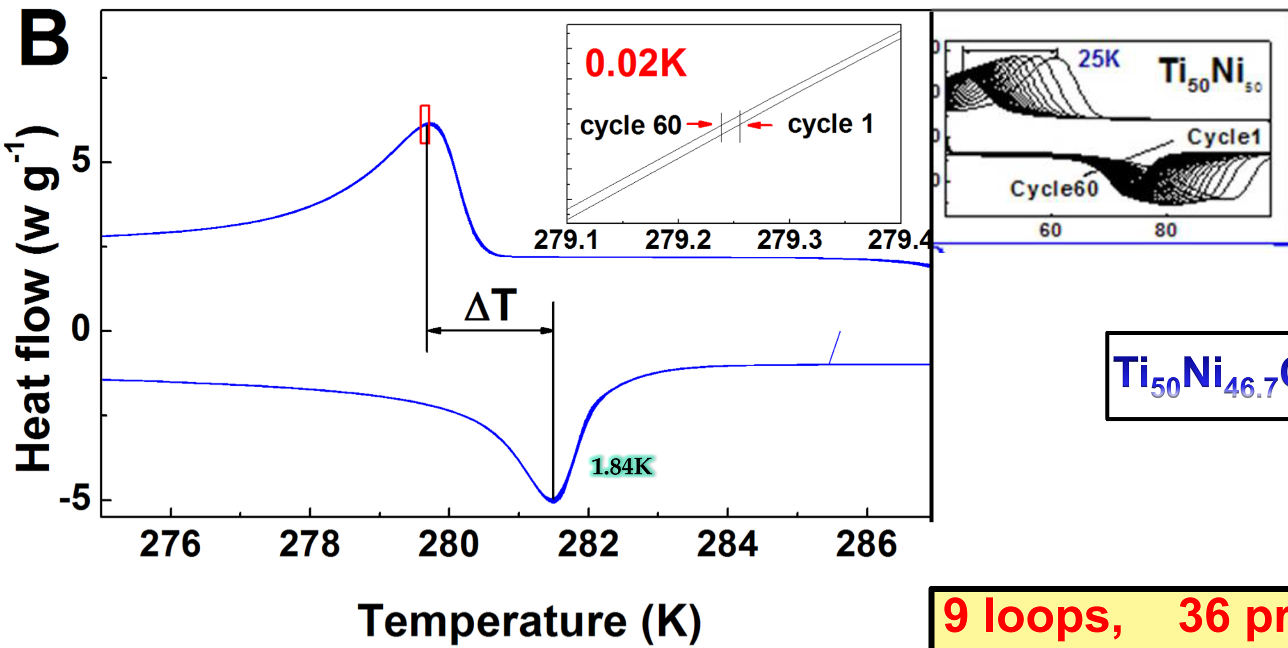
Heat treatment



Measurement: DSC



Material Performance for Synthesized Alloy



$Ti_{50}Ni_{46.7}Cu_{0.8}Pd_{0.2}Fe_{2.3}$

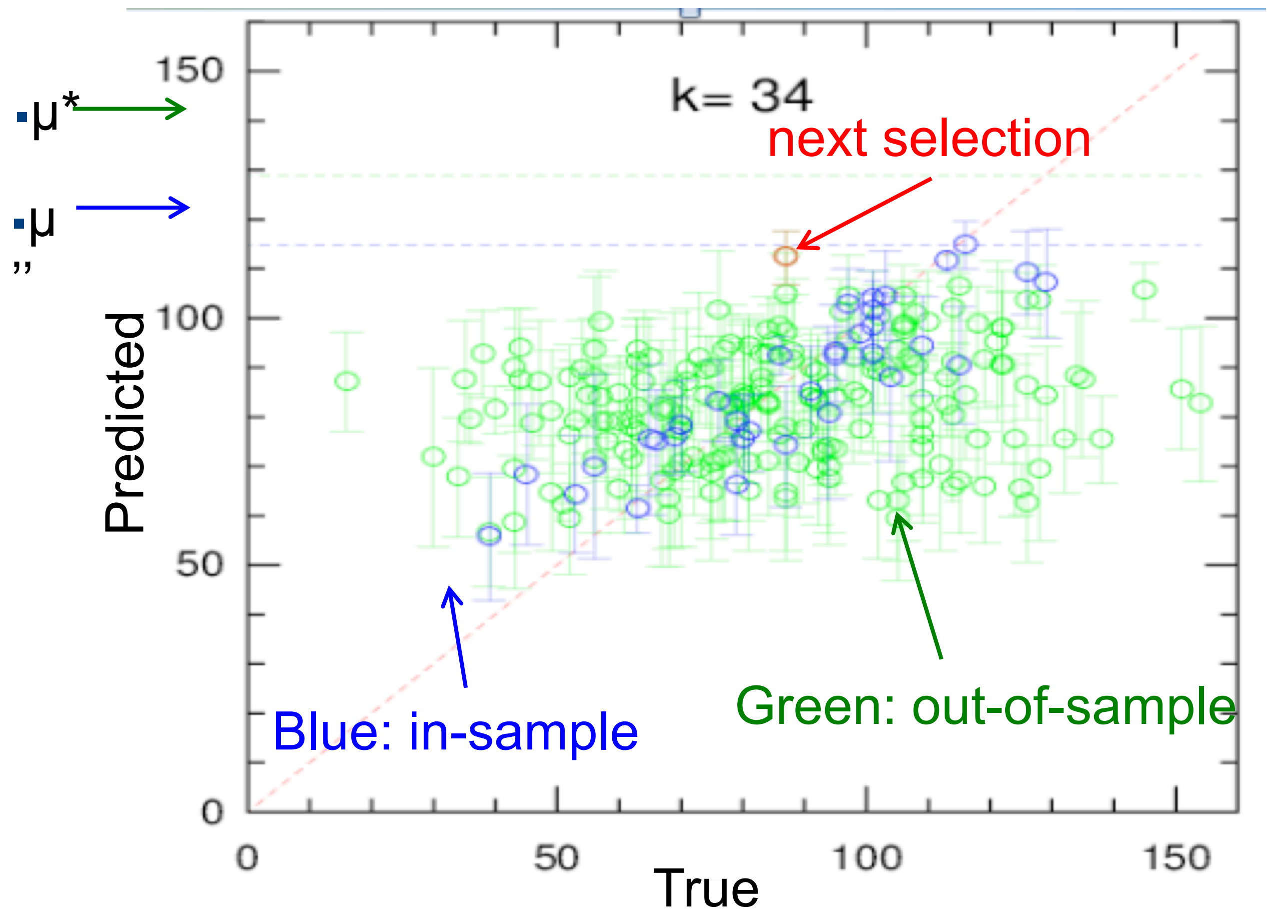
(42% improvement)

9 loops, 36 predicted and synthesized
14 better than 3.15K, p value < .001

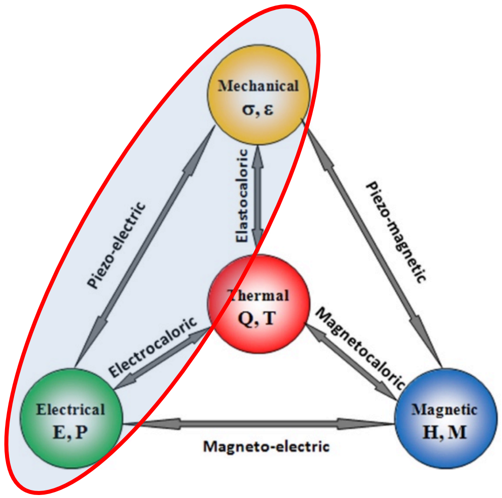
TABLE I | Five new best alloys, which were found in iterations 6 and 7, amongst 14 with the lowest ΔT. From a total of 9 iterations, which resulted in 36 new alloys, 14 had a ΔT smaller than 3.15 K, the lowest in the original training set of 22. Transformation temperature is given by the endothermic peak in the DSC curve.

Iterations	Composition	ΔT (K)	Transformation temperature (K)
6	$Ti_{50.0}Ni_{46.8}Cu_{0.9}Fe_{2.0}Pd_{0.3}$	2.64	289.95
6	$Ti_{50.0}Ni_{44.2}Cu_{1.9}Fe_{3.8}Pd_{0.1}$	2.53	243.43
6	$Ti_{50.0}Ni_{46.7}Cu_{0.8}Fe_{2.3}Pd_{0.2}$	1.84	281.77
7	$Ti_{50.0}Ni_{48.1}Cu_{0.2}Fe_{1.5}Pd_{0.2}$	2.09	301.86
7	$Ti_{50.0}Ni_{46.5}Cu_{1.1}Fe_{2.2}Pd_{0.2}$	2.32	283.79

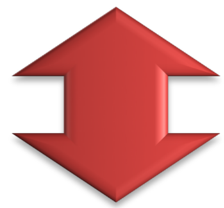
How good does the model have to be ?



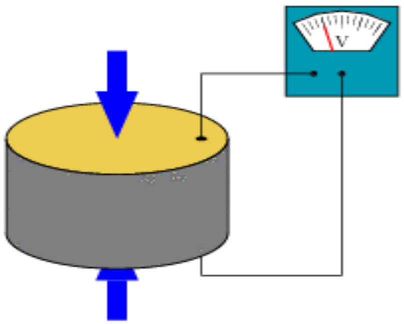
Piezoelectrics



Electrical energy



Mechanical energy



Applications

Piezoelectric Applications

Automotive
Spark Ignition
Fuel Atomization
Knock Sensors
Tire Pressure
Safety/Security Alarms
Sound Systems
Motion sensor
Flow level sensor

Consumer Goods
Telephone Ringers
Speakers
Humidifier Atomizers
Smoke Detectors
Automatic Lighting
Security Systems
Jewelry Cleaners

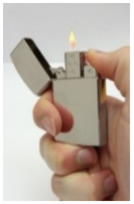
Commercial
Hydrophones
Fans
Production sensors
Counters
Security
Robotics/Toys
Game machine
Massaging

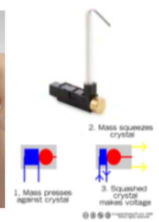
Medical
Fetal Heart Monitors
Blood Flow Diagnosis
Flow Meters/Controls
Insulin Pumps
Vaporizors / Nebulizers
Ultrasonic Surgery
Ultrasonic Imaging

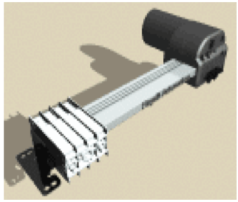
Industrial
Ultrasonic Cleaning
Ultrasonic Welding
Ultrasonic Machining
Flaw Detection
Pneumatic Valves

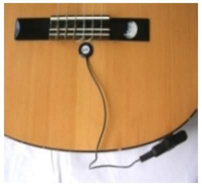
Computers
Ink Jet Printers
Disk Drive
Keyboards

Aerospace/ Defense
Sonar
Hydrophones
Ring Laser Gyros



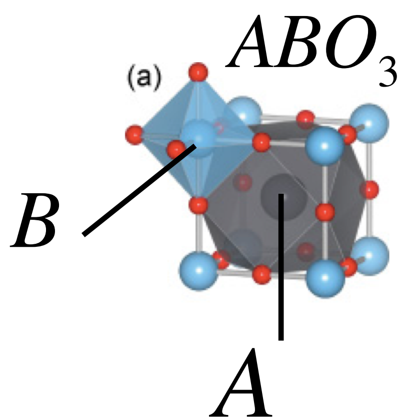


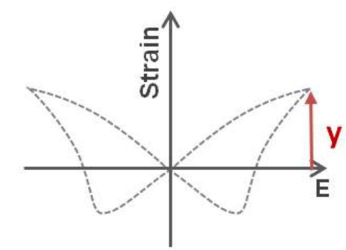




Search for BaTiO3 based solid solutions with relatively large electrostrains

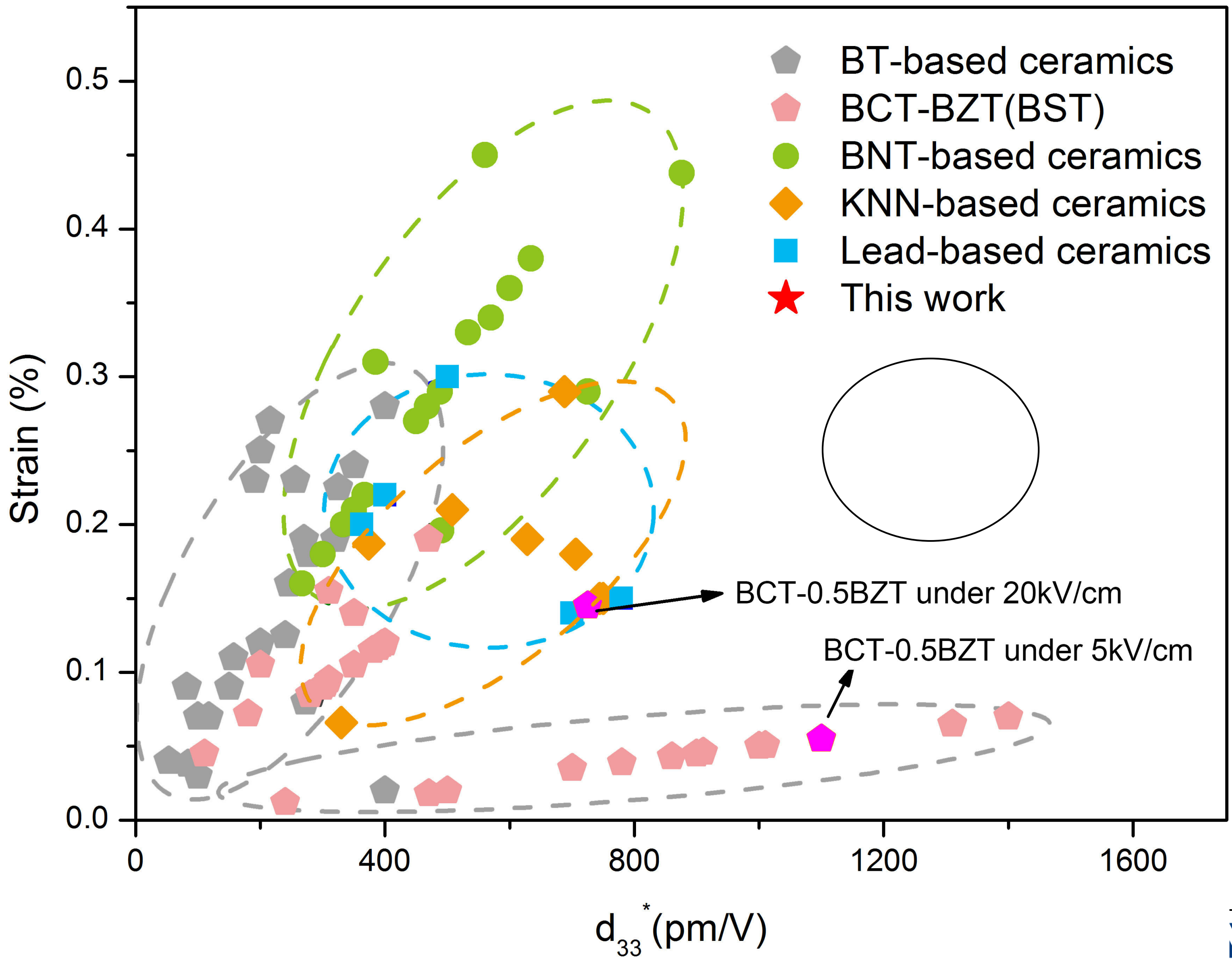
$$(Ba_{100-x-y}Ca_xSr_y)(Ti_{100-u-v}Zr_uSn_v)O_3 \begin{cases} 100-x-y \geq 60\% \quad x \leq 40\% \quad y \leq 30\% \\ 100-u-v \geq 60\% \quad u \leq 30\% \quad v \leq 30\% \end{cases}$$





Compositional control 1%

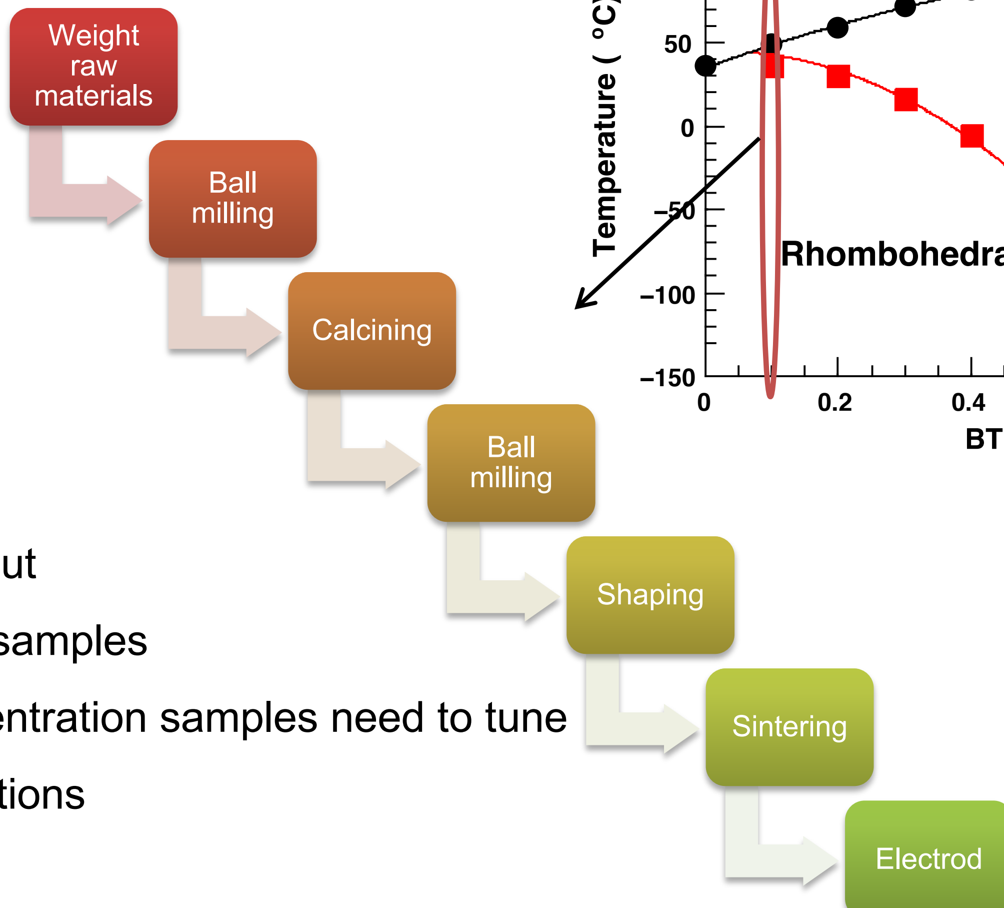
Figure of merit and target

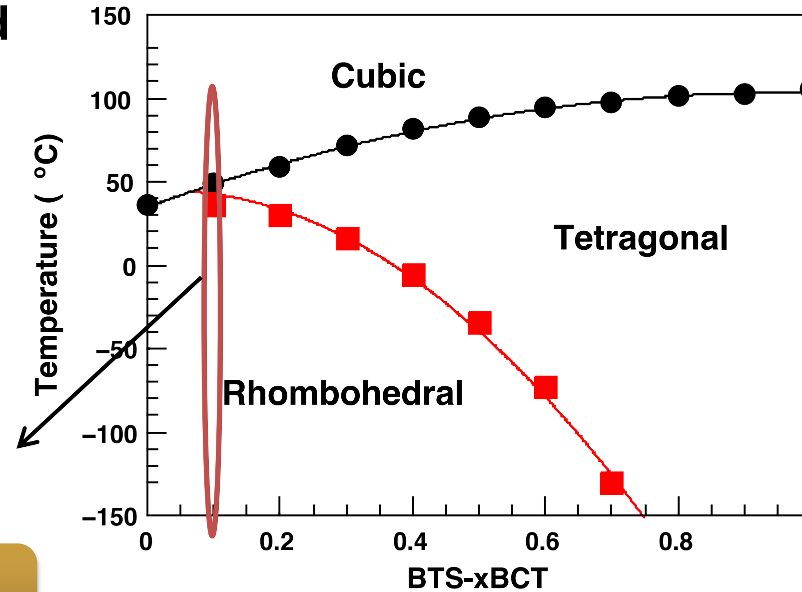


Experiments - fabrication

Conventional solid-state reaction method

Standard, but one composition in the phase diagram needs the whole procedure

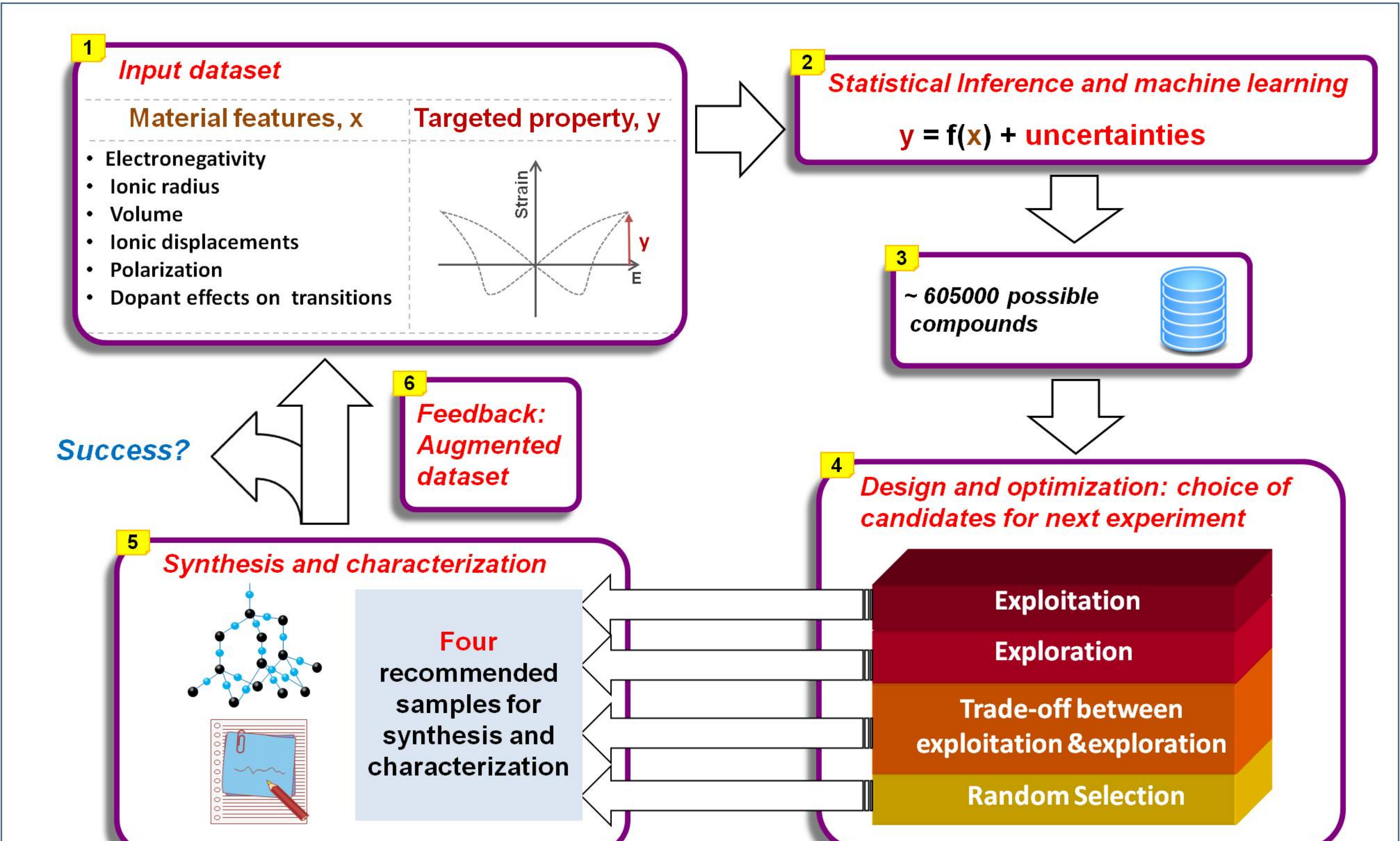




- Not high throughput
- Two days for four samples
- High dopant concentration samples need to tune the sintering conditions

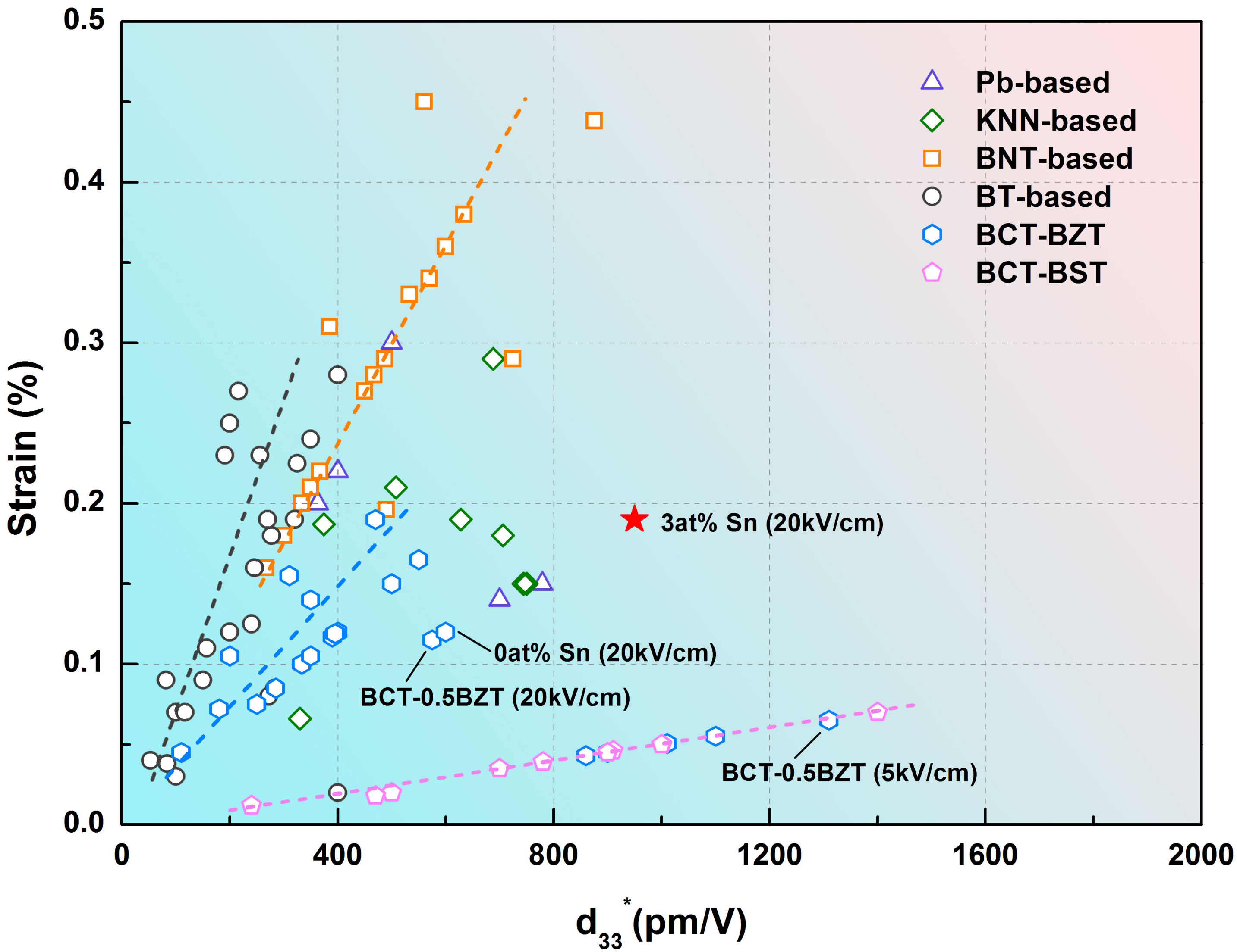
W Liu, X Ren. Physical Review Letters (2009); D Xue, et.al Applied Physics Letters (2011); C Zhou, et. al Applied Physics Letters (2013)

Experimental Comparison of design strategies : Search for BaTiO3-based large electrostrains

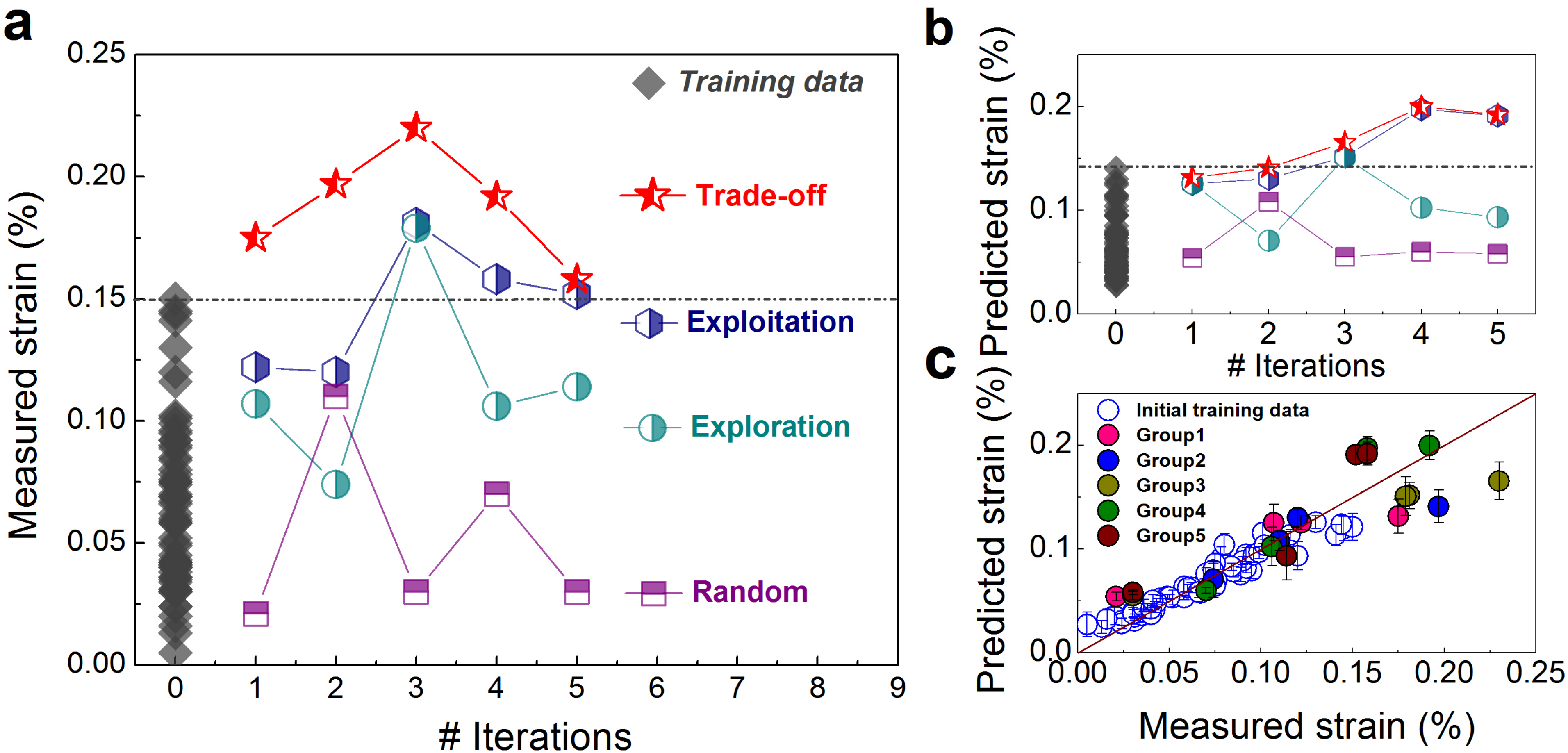


Relative Figure of Merit

$(Ba_{0.84}Ca_{0.16})(Ti_{0.90}Zr_{0.07}Sn_{0.03})O_3$



Comparing outcome to predictions

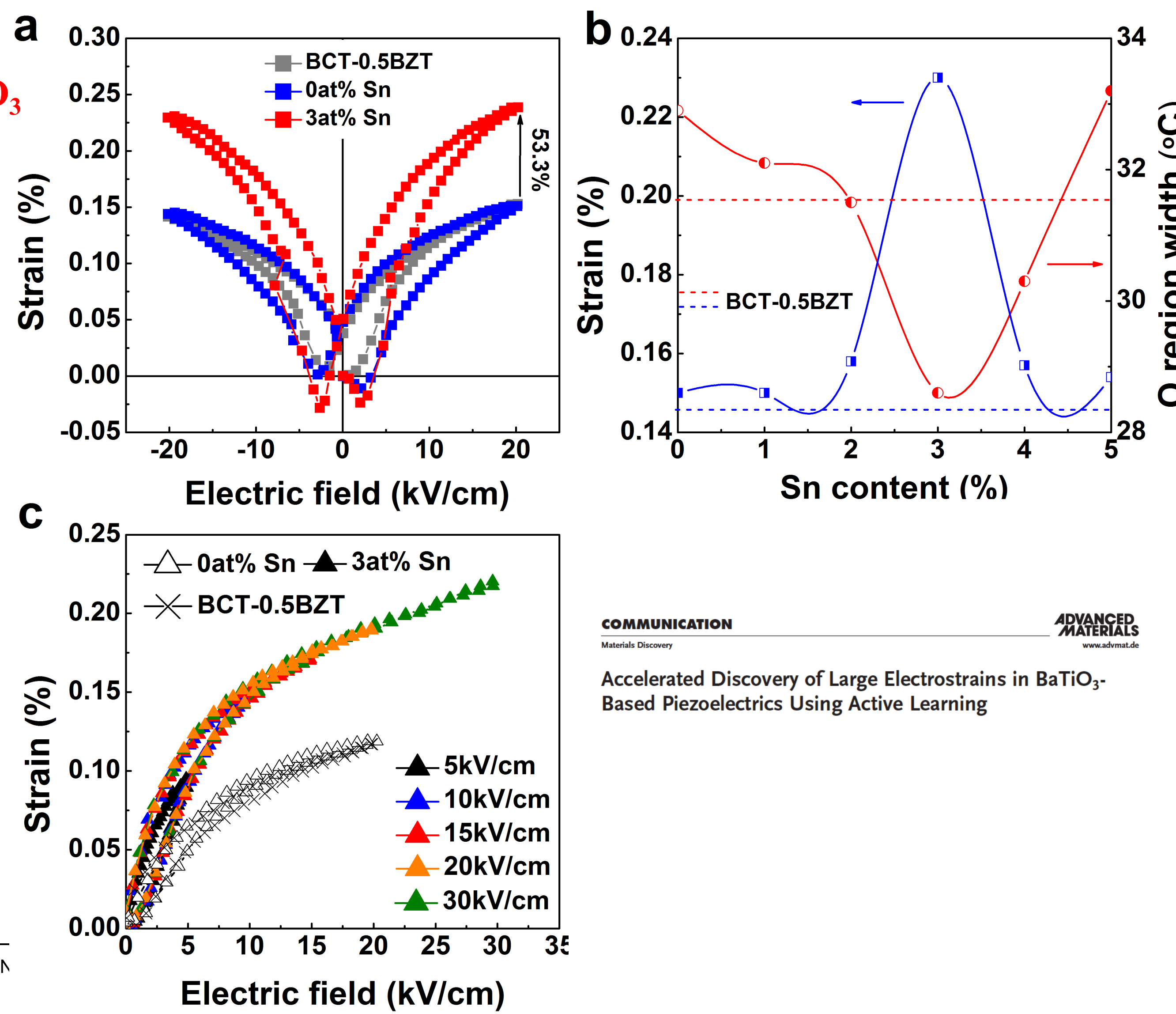


Comparison of BCT-BZT based piezoelectrics

$(Ba_{0.84}Ca_{0.16})(Ti_{0.90}Zr_{0.07}Sn_{0.03})O_3$

$(Ba_{0.84}Ca_{0.16})(Ti_{0.90}Zr_{0.10})O_3$

$(Ba_{0.84}Ca_{0.15})(Ti_{0.90}Zr_{0.10})O_3$



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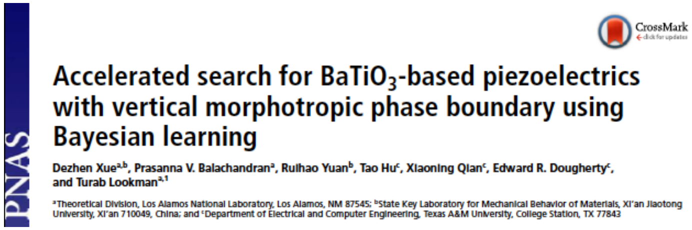
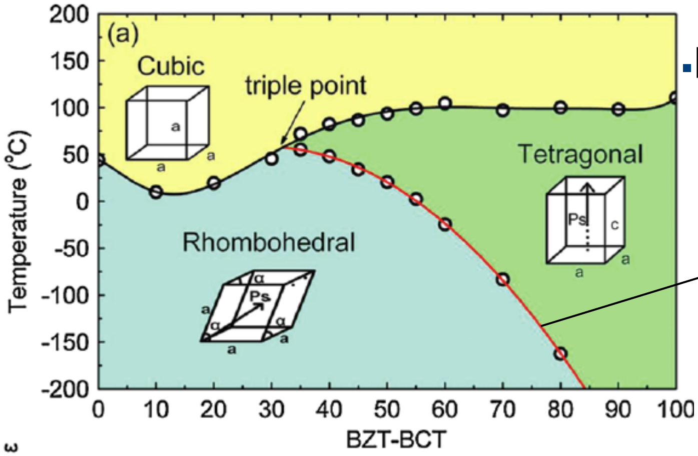
Accelerated Discovery of Large Electrostrains in $BaTiO_3$-Based Piezoelectrics Using Active Learning

Example: Importance of knowledge

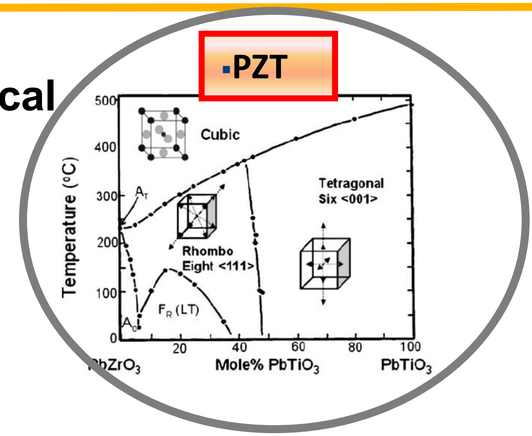

Accelerated search for $BaTiO_3$-based piezoelectrics with vertical morphotropic phase boundary using Bayesian learning

Dezhen Xue[a,b], Prasanna V. Balachandran[a], Ruihao Yuan[b], Tao Hu[c], Xiaoning Qian[c], Edward R. Dougherty[c], and Turab Lookman[a,1]

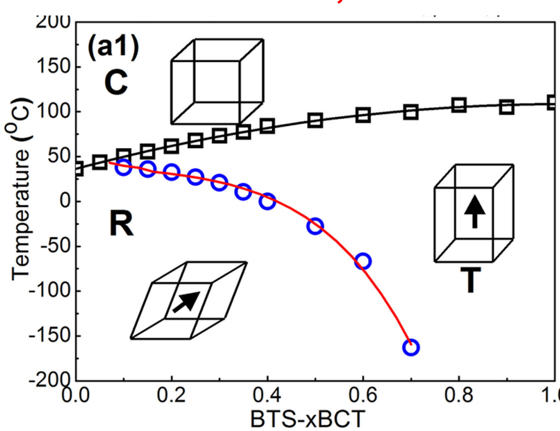
[a]Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545; [b]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China; and [c]Department of Electrical and Computer Engineering, Texas A&M University, College Station, TX 77843



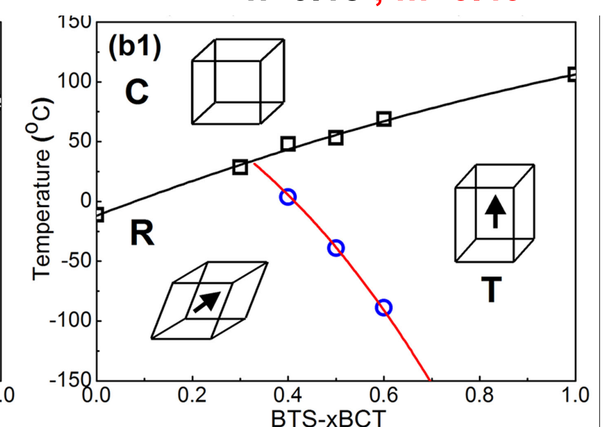
- Design criterion: Vertical



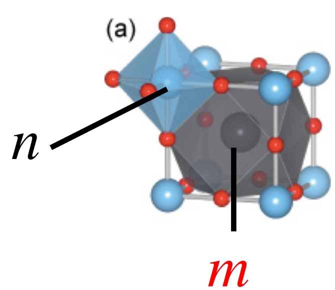
- n=0.12 ; m=0.30



- n=0.18 ; m=0.40

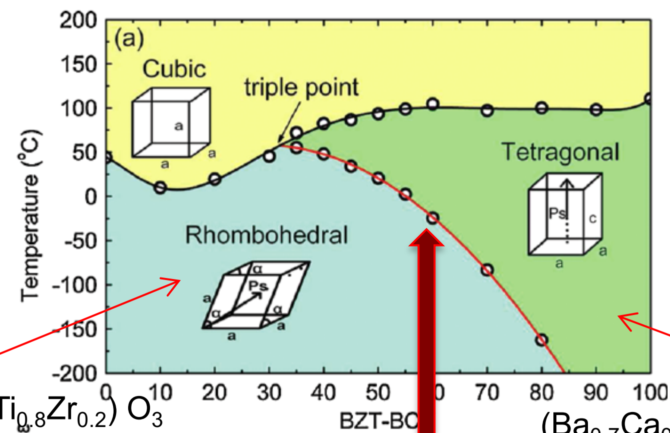


A_n - B_m



- Q: What combination of m,n and chemistries (Al, Li, …) will optimize phase boundaries, response?

Approach



$Ba(Ti_{0.8}Zr_{0.2})O_3$

$(Ba_{0.7}Ca_{0.3})TiO_3$

(111)

$$f_R = \frac{1}{2}a_2(\tau - \tau_C)p_R^2 + \frac{1}{6}\left(a_6 - \frac{1}{9}a_6' - \frac{1}{27}a_6''\right)p_R^6$$

(100)

$$f_T = \frac{1}{2}a_2(\tau - \tau_C)p_T^2 + \frac{1}{6}(a_6 - a_6')p_T^6$$

At MPB $f_R = f_T \Rightarrow \tau = f(\tau_C, a_2, a_6, .., p_R, p_T)$

Learning from theory + data

x(Ba1-mCam)TiO3−Ba(ZrnTi1-n)O3

$x(Ba_{1-m}Ca_m)TiO_3-Ba(Zr_nTi_{1-n})O_3$

18%< m < 50%; 15% < n < 30%

(1200 phase diagrams)

- Features:
  - Order parameters: Polarization, Strain

$$\Delta V = V_T - V_R \qquad u_T, u_R$$

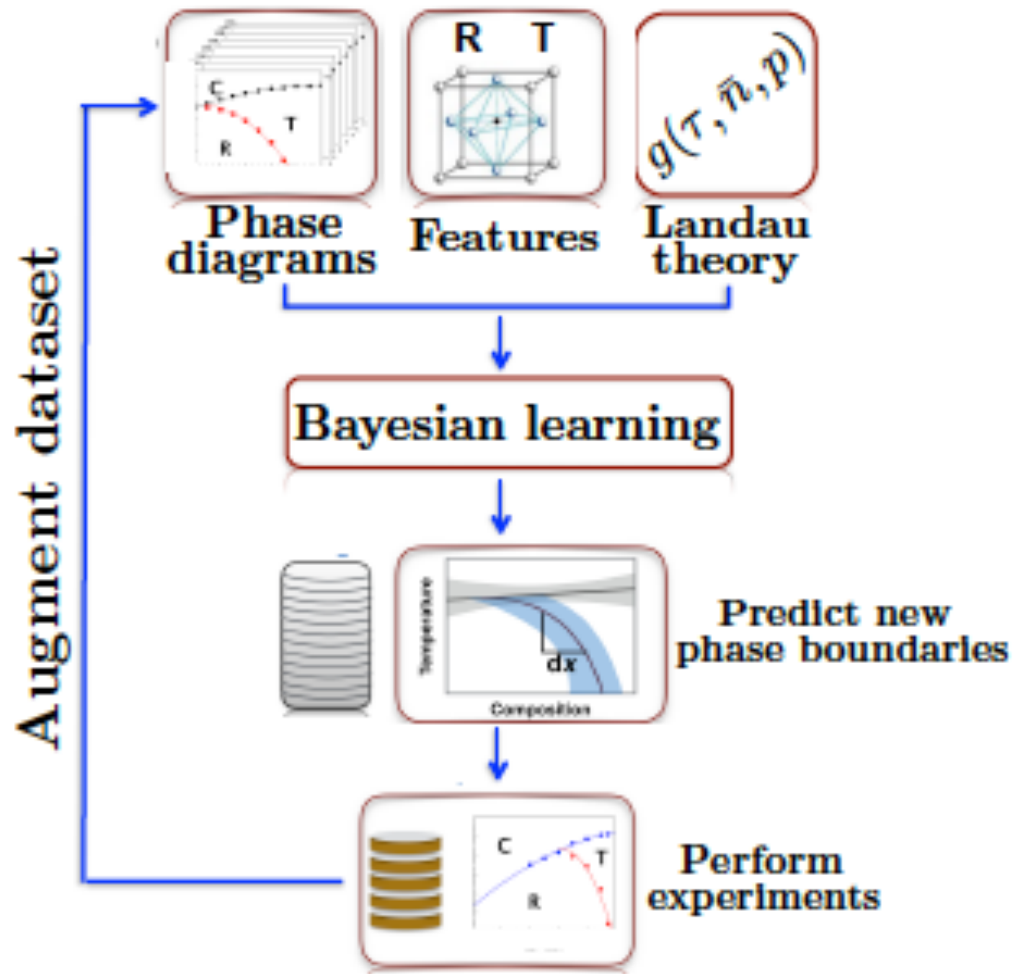
$$t_f = \frac{R_A^T + R_o}{R_B^R + R_o} \qquad r_{eff\_nucl} = \frac{A_{enc_T}}{B_{enc_R}} \qquad r_{elec\_neg} = \frac{A_{en_T}}{B_{en_R}}$$

- Training data: 19 phase diagrams

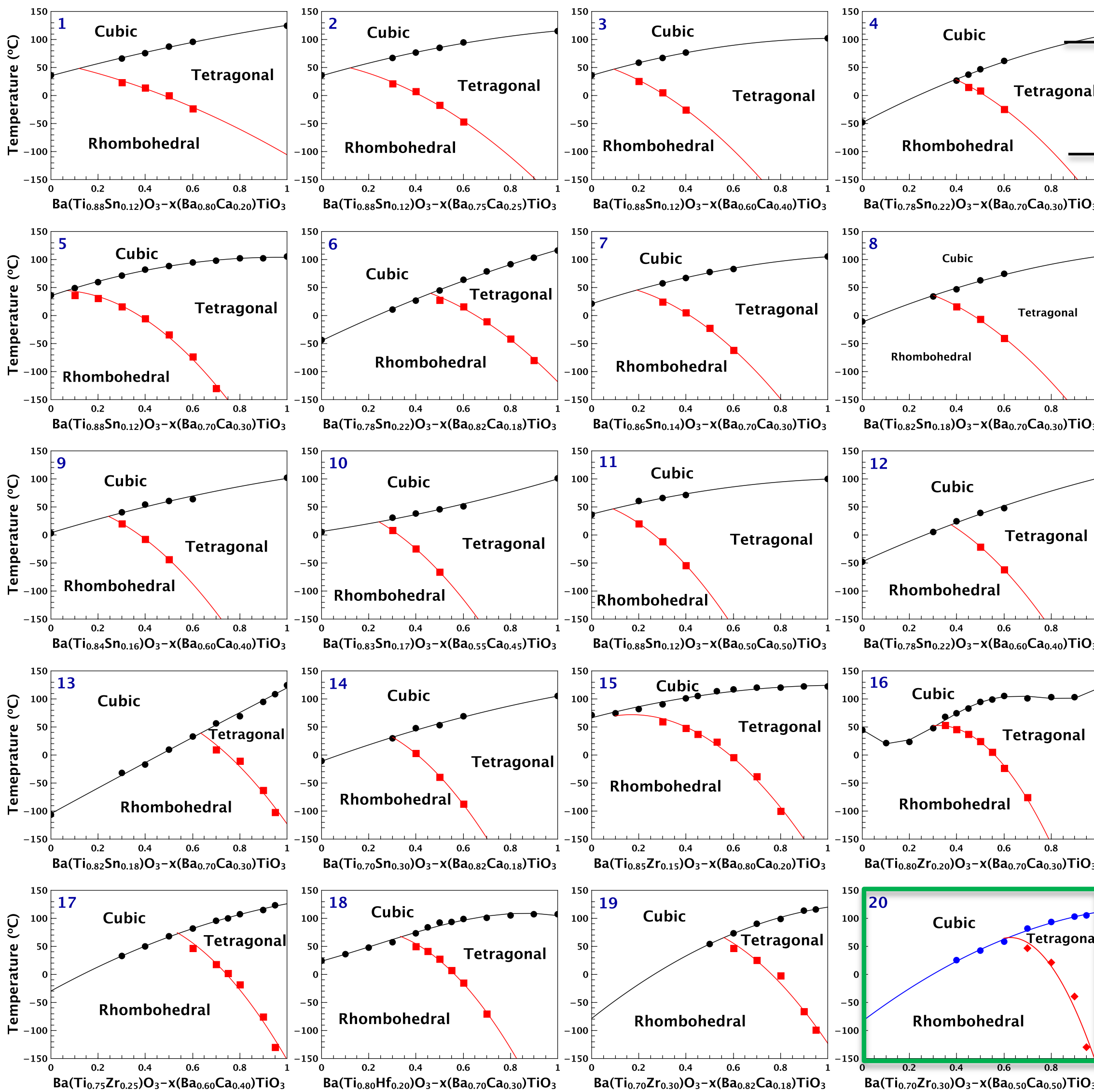
$$\tau = f(\tau_C, a_2, a_6, .., p_R, p_T)$$

- Prior distribution subject to constraints

- Take samples from posterior



Data



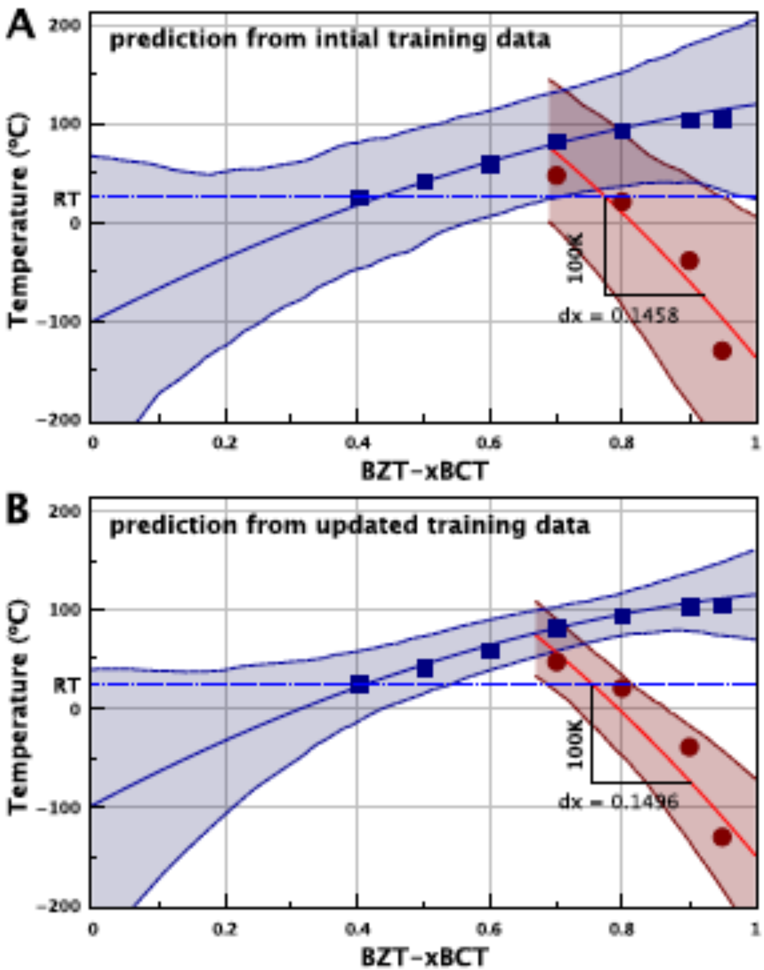
$\rightarrow \tau_{\mathrm{PF}}$

$\rightarrow \tau_{\mathrm{MPB}}$

(both show composition dependence)

➤ ***New***

Predictions/ synthesis from model + data

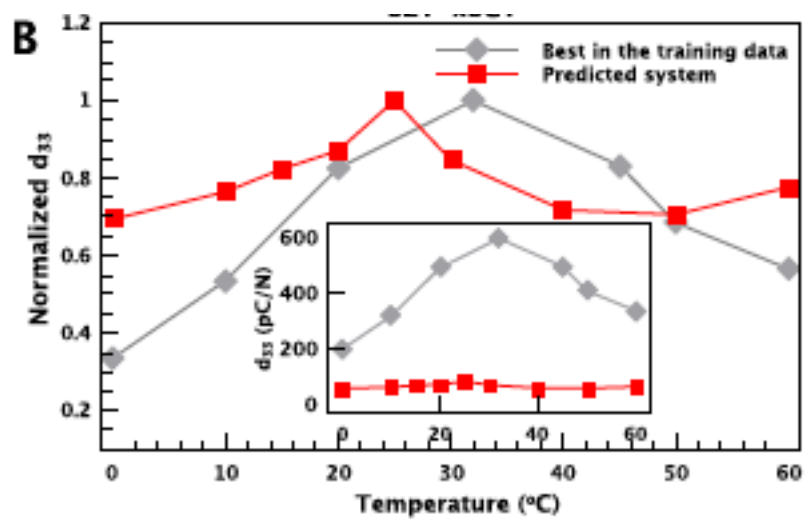


Best in the training data:

$Ba(Zr_{0.2}Ti_{0.8})O_3 - (Ba_{0.7}Ca_{0.3})TiO_3$

New Prediction:

$Ba(Zr_{0.3}Ti_{0.7})O_3 - (Ba_{0.5}Ca_{0.5})TiO_3$



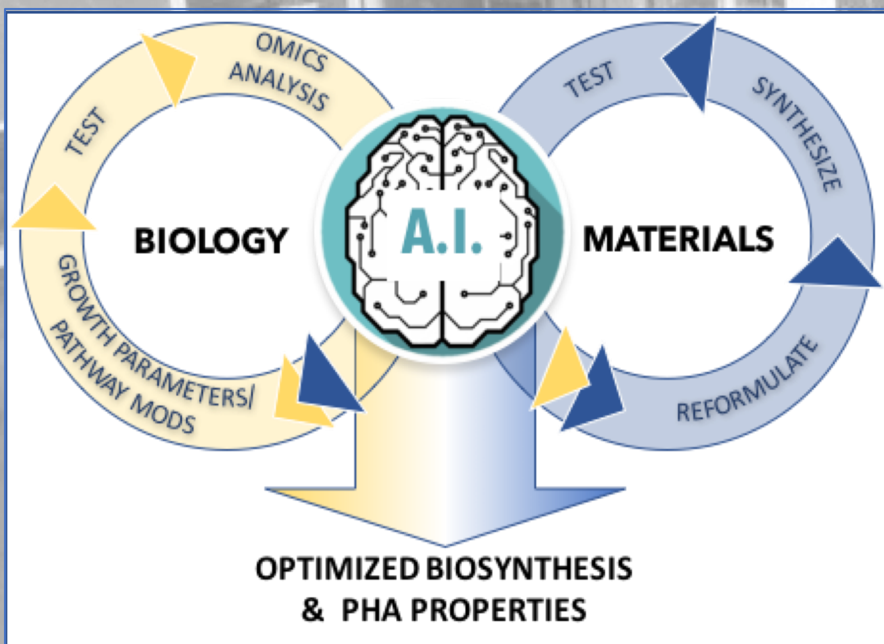
Xue *et al.*, PNAS, 2016

Challenges – Path forward

- No free lunch theorem ! (Wolpert, 98)
- Integrate physics models
- Guiding principles for different classes of problems (materials, ..)

BioManufacturing with Intelligent Adaptive Control

BIOMANIAC



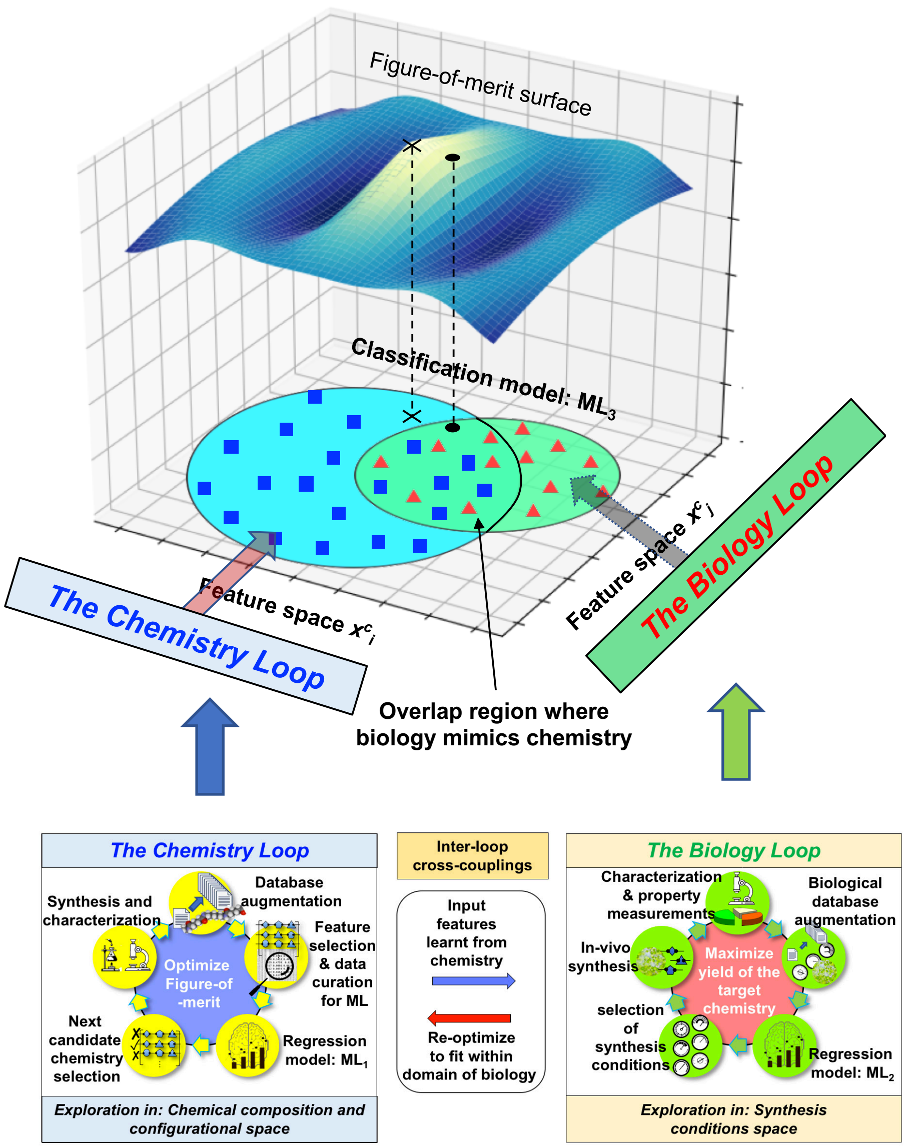
LASL's **MANIAC** (***M****athematical* ***A****nalyzer,* ***N****umerical* ***I****ntegrator, and* ***C****omputer* or ***M****athematical* ***A****nalyzer,* ***N****umerator,* ***I****ntegrator, and* ***C****omputer* was an early computer built under the direction of Nicholas Metropolis, 1952

What Problem are we Trying to Solve?

- Plastics–synthetic polymers made from petrochemicals–have revolutionized our society.
- However, plastics are over-engineered for durability, and plastic pollution is now a scourge on our planet.
- We propose to help solve this problem with an *innovative process* to discover, design, and develop new biopolymers with improved functionalities, balancing durability with faster degradability in the environment.
- Use biology as a template for new chemistries.

The Plastic Lifecycle. *Top: Past: Cradle to Grave. Plastic from petroleum is used for most packaging, but ends up in landfills or in the environment. Bottom: Future: Cradle to Cradle. Algae can be used to produce bio-based plastics. Along with improved recycling methods (e.g. P&G's Head & Shoulders shampoo bottle made from pelletized beach plastic) biodegradable compostable bioplastic can be broken down into basic molecules that can be captured and re-used as nutrients in agriculture.*

APPROACH



- A model or recipe that will predict the synthesis conditions/chemistries to make **polymers with targeted performance** from the biology or chemistry routes with given confidence levels.
- **A general approach that allows for efficient exploration** of vast chemical spaces and synthesis conditions using ML to guide chemistry and/or biology based synthesis routes
- **Novel, degradable biopolymers** (with a favorable combination of other properties, e.g., breathability, durability, mechanical strength) synthesized via the proposed biosynthesis route