GreenALM

Virtual Psi-k GreenALM Hands-on Tutorial 2021

Accelerated material design based on DFT, experiment and machine learning

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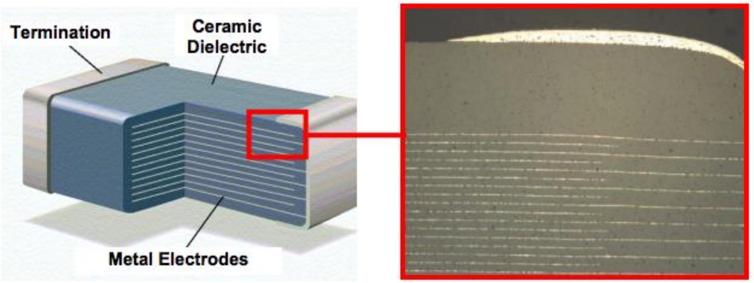
14.10.2021

→ High-performance materials require intelligent materials design

Mobility

Energy

Tooling



Electronics

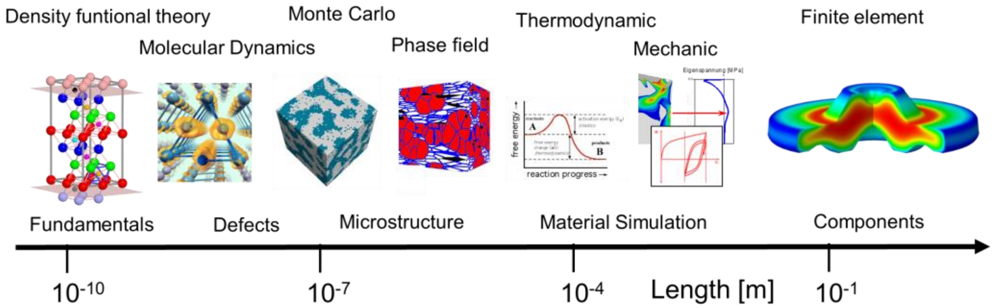
ICME:

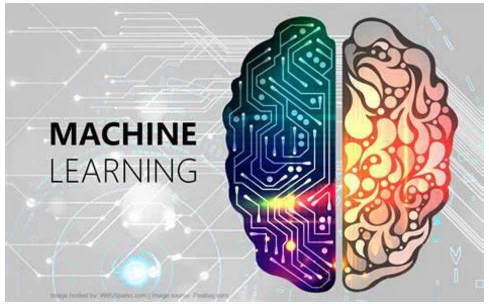
Connect physics - based models at various length scales (e.g., atomistic simulation, dislocation modeling, thermodynamic continuum modeling) to predictively model materials

Material informatics:

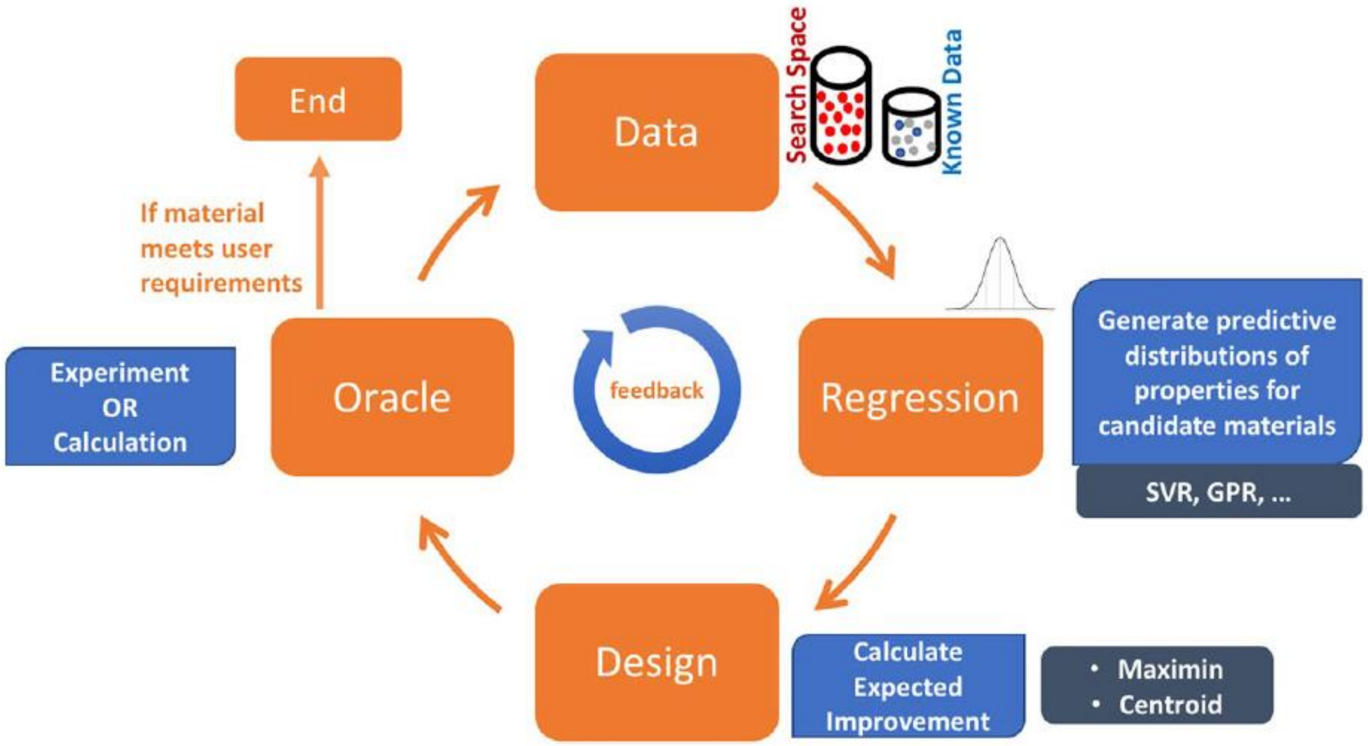
Understand materials using data and algorithms with machine learning as a key tool

Joanne Hill , Gregory Mulholland , Kristin Persson, Ram Seshadri , Chris Wolverton , and Bryce Meredig, MRS BULLETIN, 41, 2016, 399





Workflow: Lookman loop



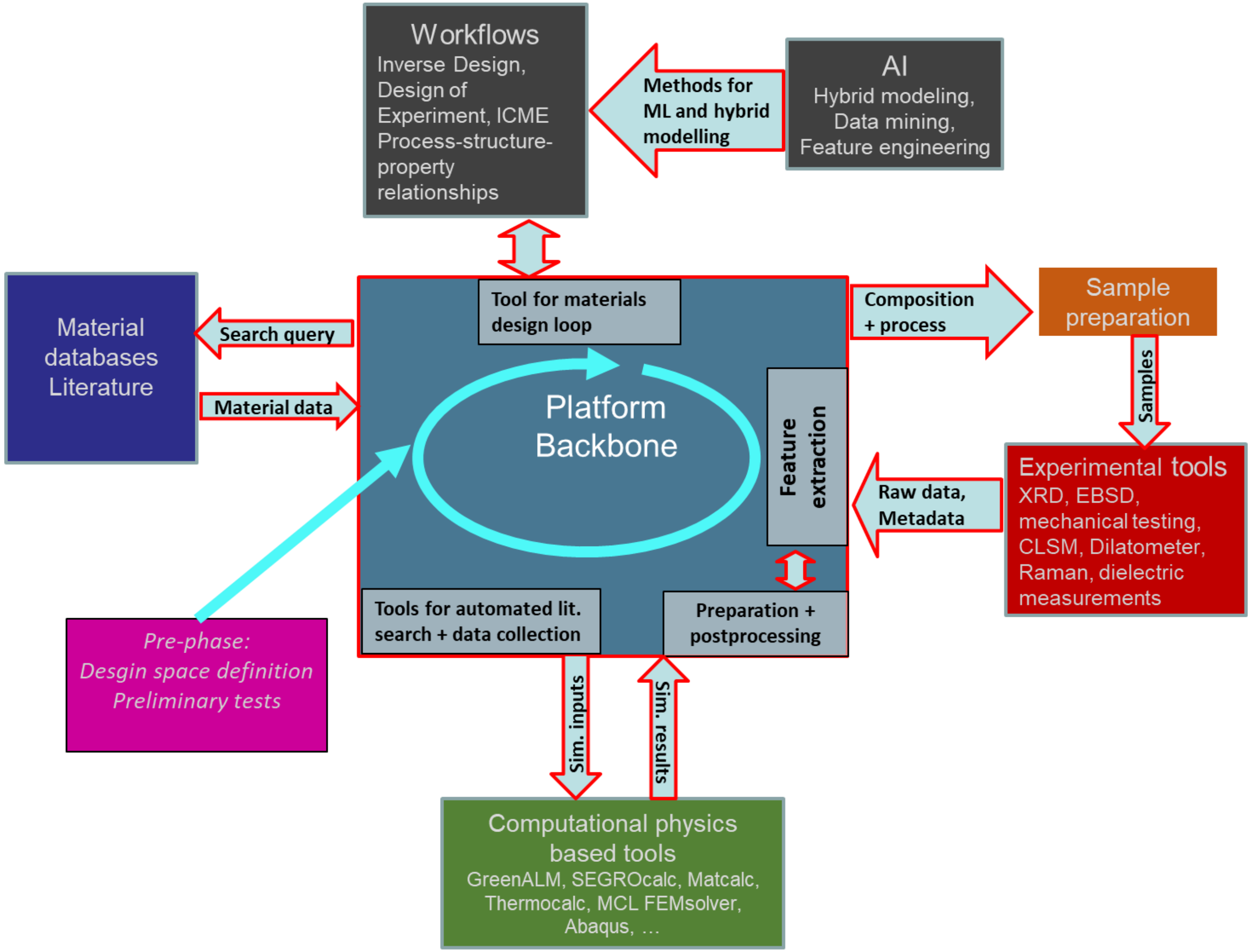
- Loop through data generation, data learning, prediction of best material/device and validation.
- Learn data as they are created.
- Move efficiently through complex design spaces.
- Obtain better materials with well-defined workflow

DOI:10.1038/s41598-018-21936-3

Implementation of accelerated materials design loop at MCL

Elements of the accelerated materials design framework at MCL

- Pre-phase: Desgin space definition, preliminary tests
- Automated access to material databases and literature
- AI based tools for materials design loop … next material to be synthesized
- Synthesis
- Experimental characterization
- Computational physics based tools: GreenALM, VASP, effective Hamiltonians, SEGROcalc, Thermocalc, FEM solvers,

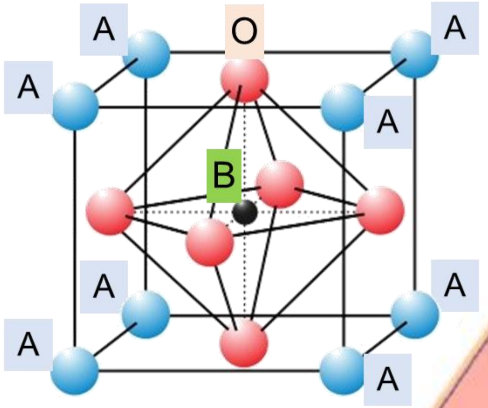


- Typical chemical formula ABO_3, e.g. $BaTiO_3$
- Huge design space: combinatorial bottleneck.
- **Objective**: Ferroelectric perovskites with large piezoelectric and electromechanical coupling coefficients

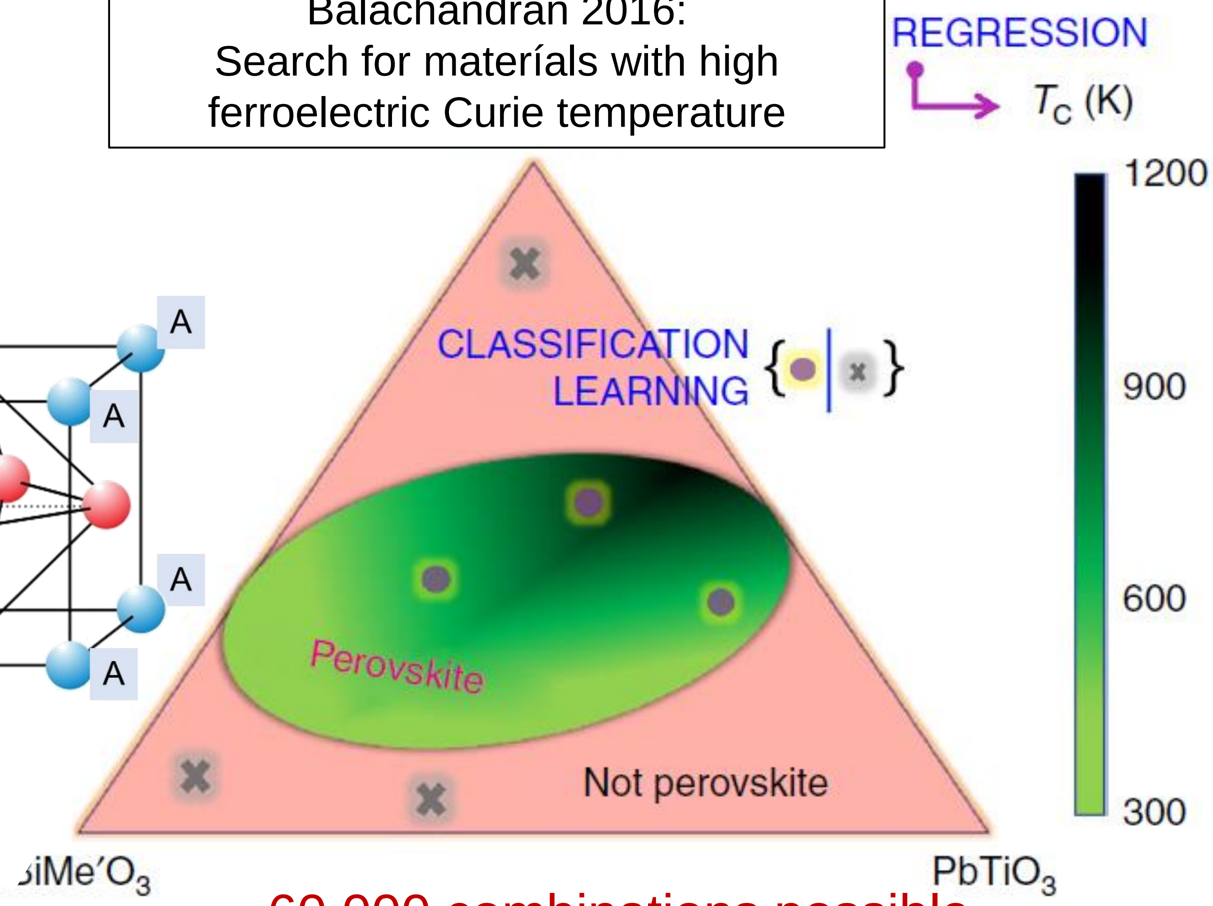
$(A_{1-x-y}A'_xA''_y)(B_{1-j-k}B'_jB''_k)O_3$

Where

A (2+) = Ba, Ca, Sr
A' (3+) = Bi, Ce, Dy, Er, Eu, Gd, La, Nd, Pr, Sm
A" (1+) = Ag, K, Li, Na
B (4+) = Ce, Hf, Os, Pd, Re, Rh, Sn, Ti, V, Zr
B' (2+ or 3+) = Co, Fe. Ga, Mg, Mn, Sb, Tb, Yb, Zn
B" (5+ or 6+) = Mo, Nb, Sb, Ta, W



Balachandran 2016:
Search for materíals with high ferroelectric Curie temperature



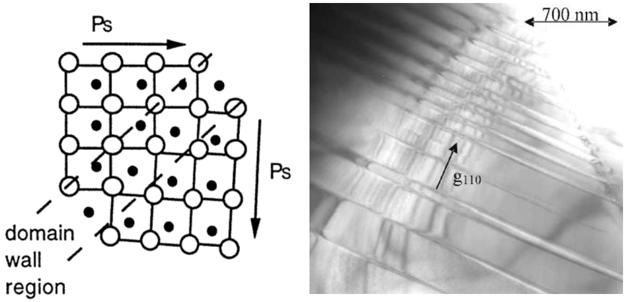
60.000 combinations possible, not even 1% explored

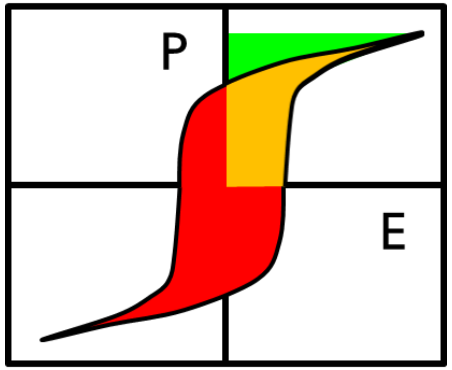
DOI: 10.1038/s41467-018-03821-9

Perovskite ferroelectrics with high energy density

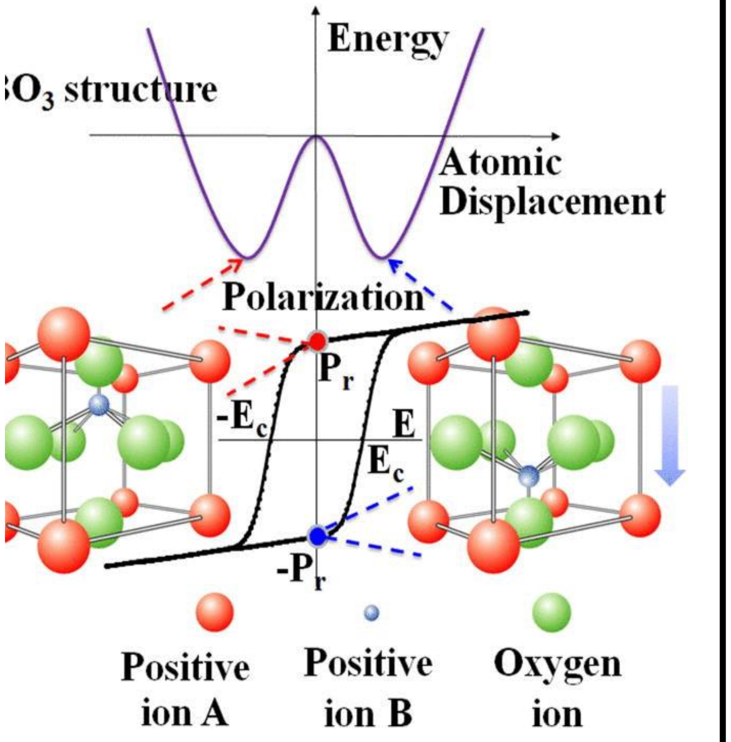
Ferroelectrics

Cooperative long-range cation displacement





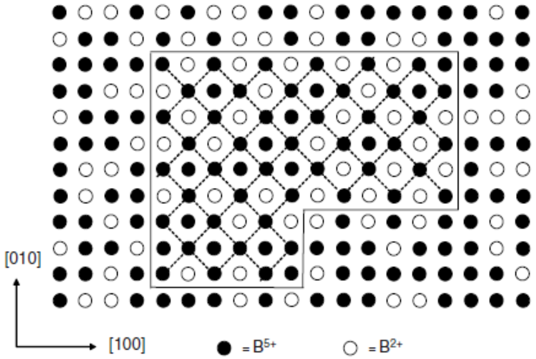
Perovskite structure

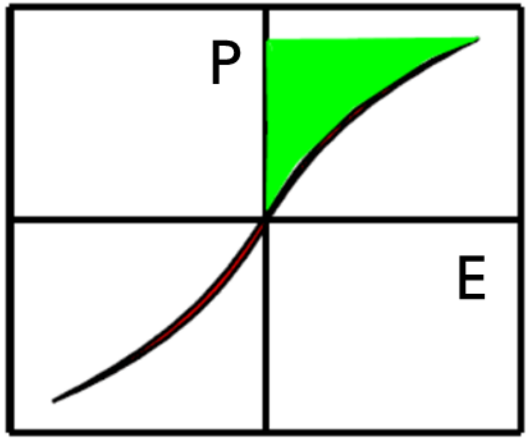


A-site	**B-site**
large cation	medium-sized cation
Ba^{2+}, Pb^{2+}, Bi^{3+}, La^{3+}…	Ti^{4+}, Zr^{4+}, Nb^{5+}, Yb^{3+}…

Relaxors

Disruption of long-range correlation

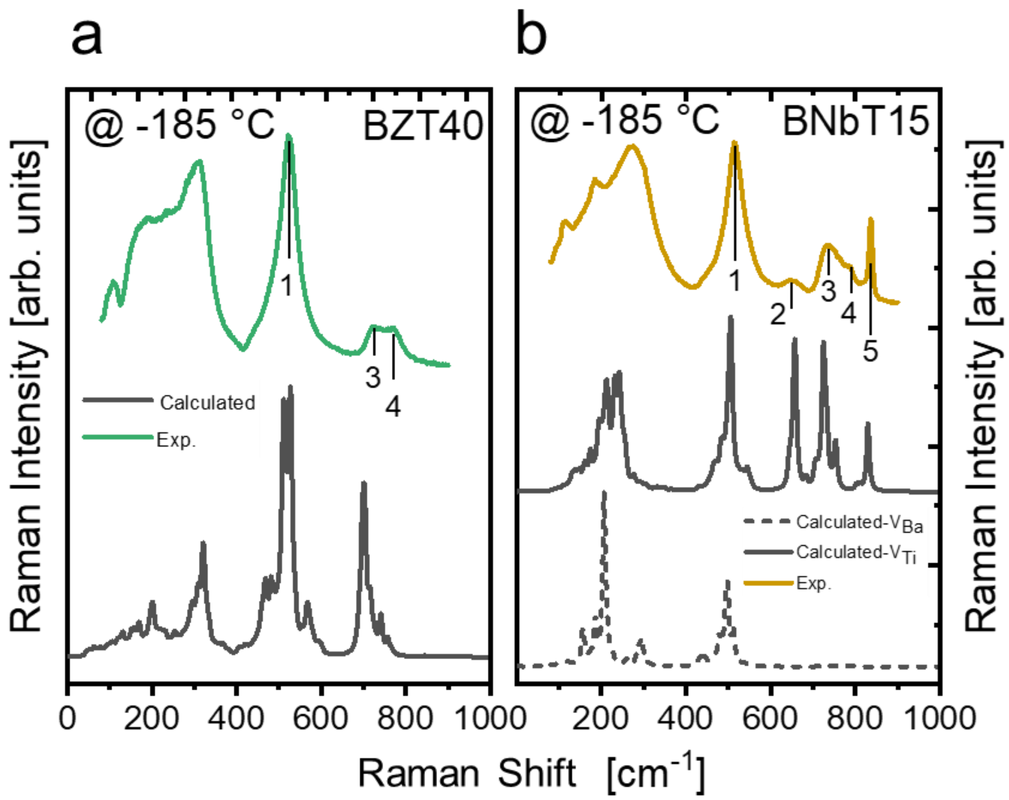




- Atomic-level characterization **Raman + DFT**
  - High-throughput synthesis (spin coating)
  - Characterization with **Raman** and XRD
  - DFT + SpheRaE: Prediction of spectra for different defects/local defect arrangement

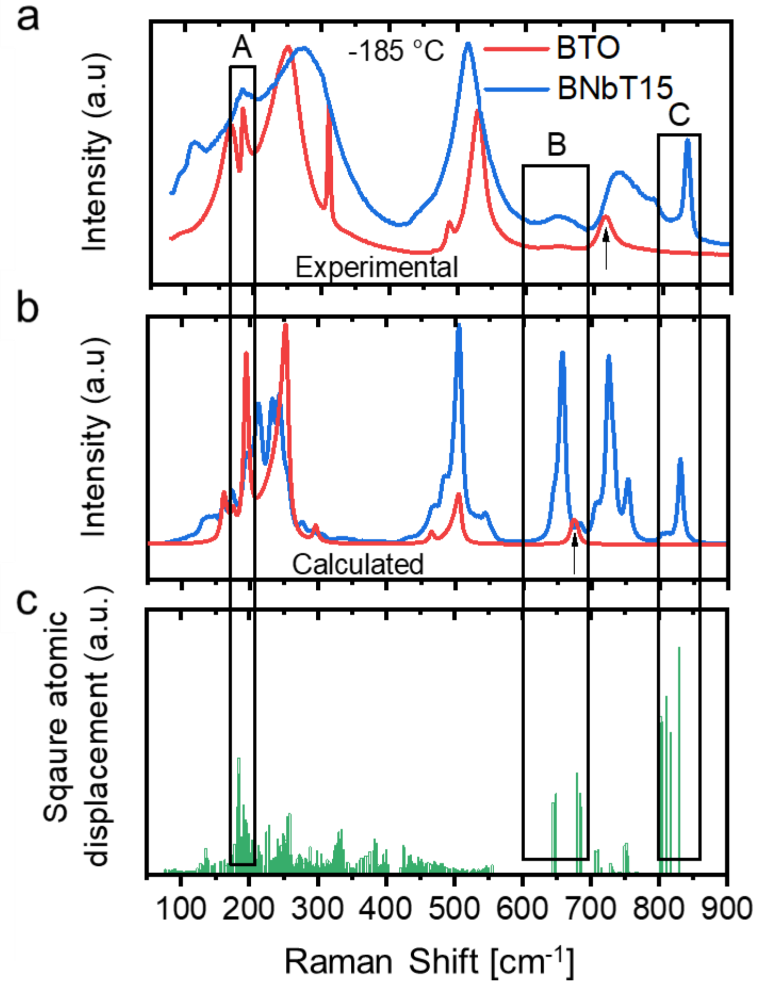
Atomic level characterization of functionally active part

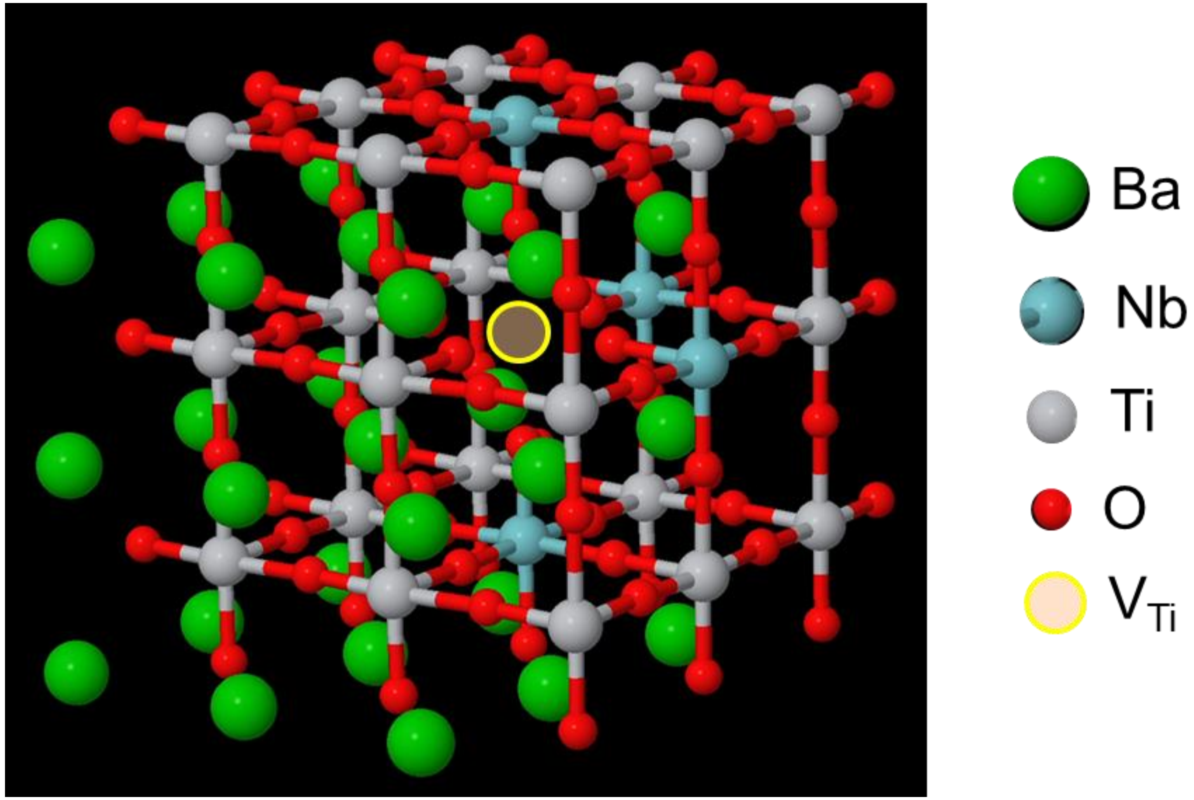
Example of Ba(NbTi)O_3 and Ba(ZrTi)O_3



1) Popov et al 2020, https://doi.org/10.1038/s41524-020-00395-3

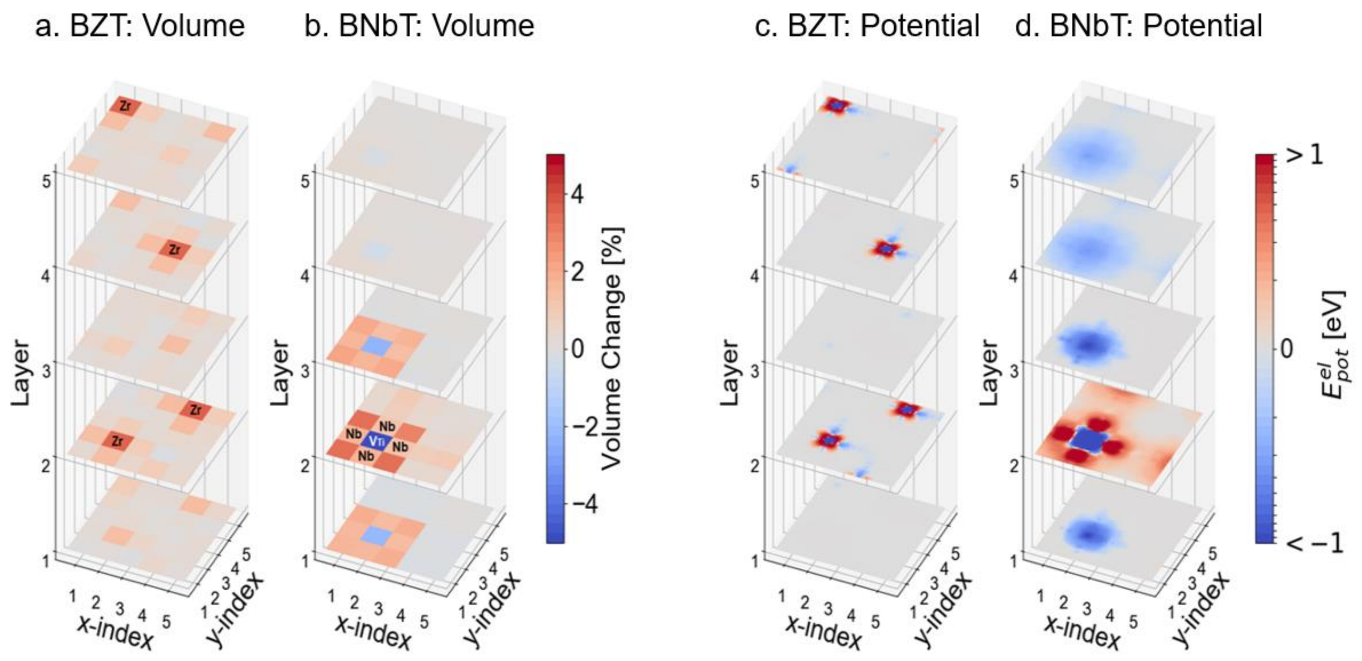
$Ba(NbTi)O_3$



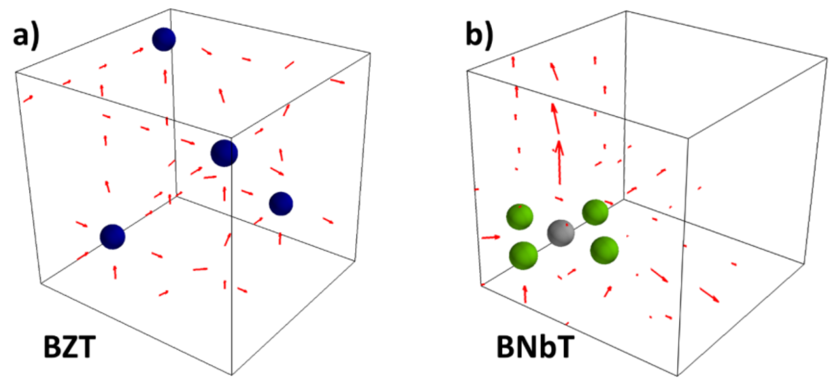


1) Veerapandiyan et a, submitted to Advanced Electronic Materials

- Impact of Zr and Nb on local dipole moments



Local dipole changes induced by doping BT

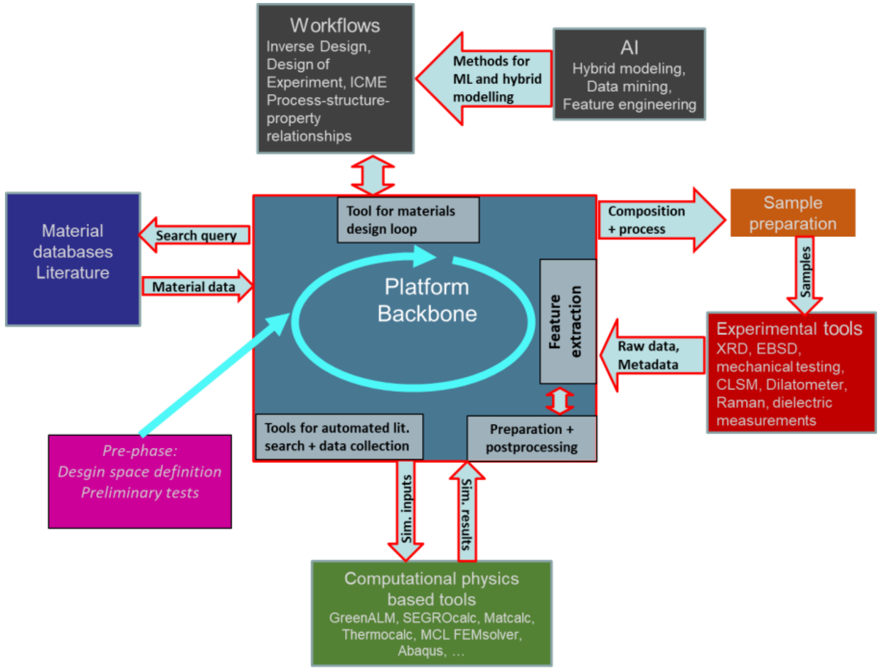


1) Veerapandiyan et a, submitted to Advanced Electronic Materials

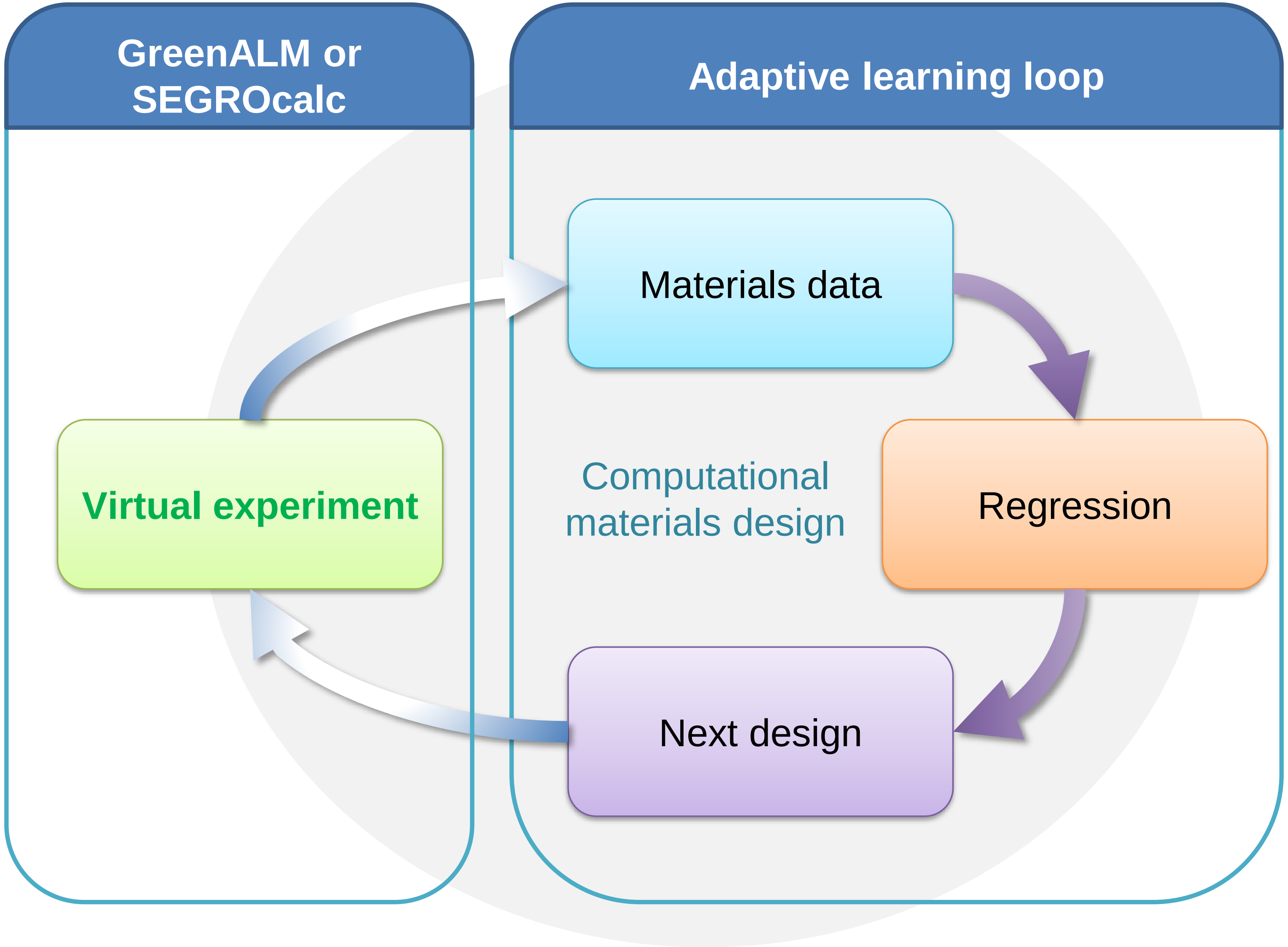
Perovskites: Materials design workflows

- ❑ High-throughput synthesis (sol-gel deposition)
- ❑ Characterization
  - ❑ XRD, Raman, HR-TEM
  - ❑ Atomistic modeling: DFT
- ❑ Physical modeling: DFT based effective Hamiltonians
- ❑ Machine learning

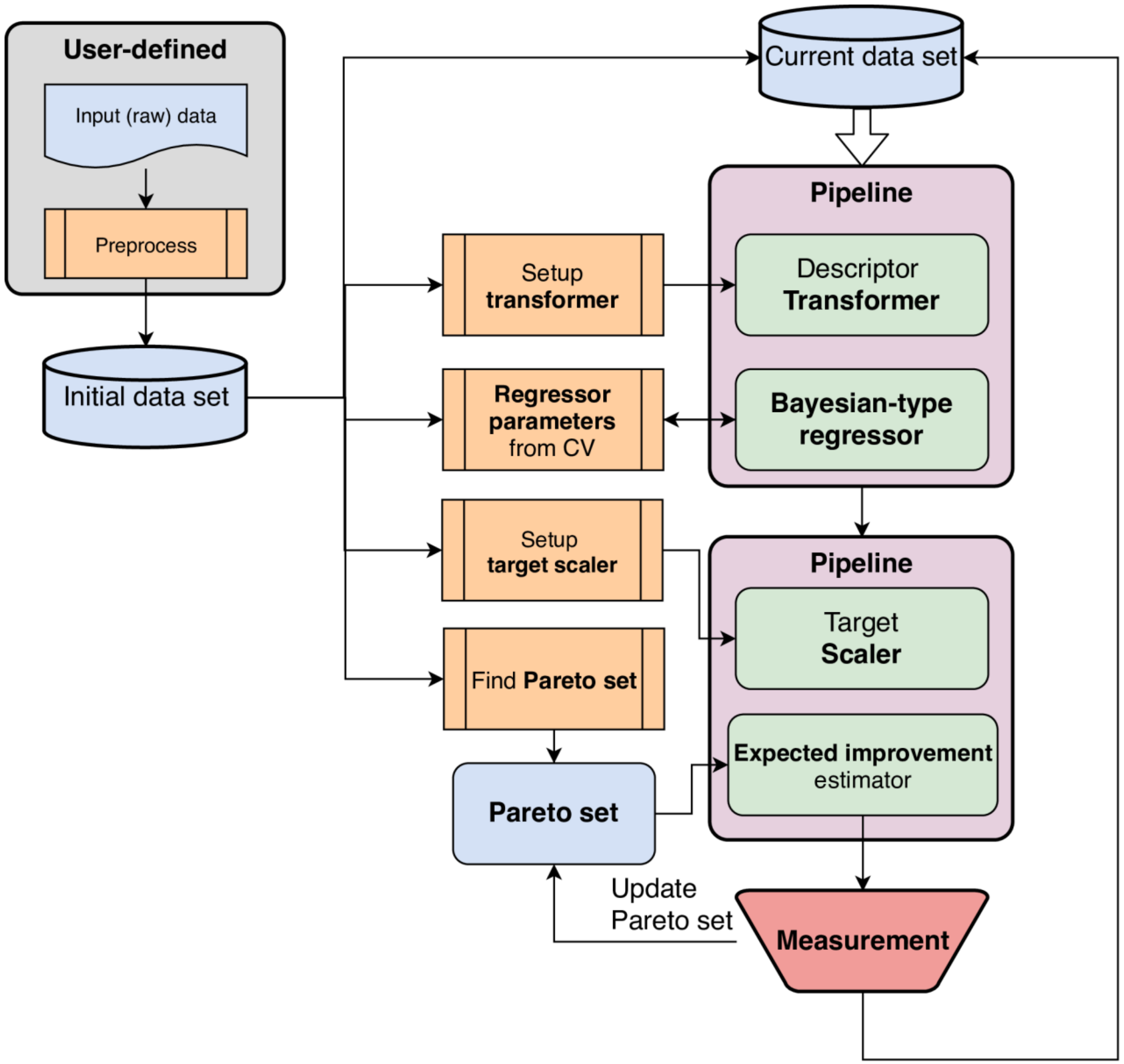
Perovskite-based materials with exceptional energy storage capability



Adaptive design of alloy materials

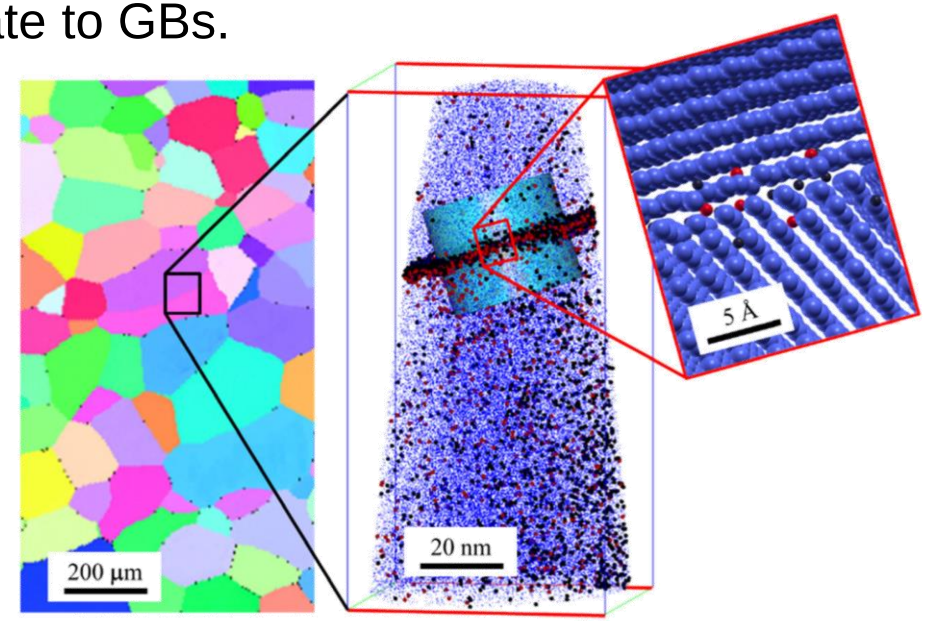


Adaptive learning workflow in practice

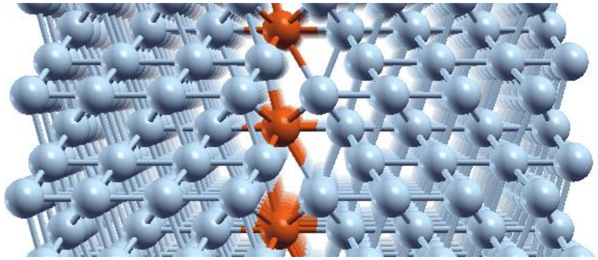


Task: Find heat treatment that increases GB cohesion for Fe containing C, B, and N as impurities.

- **Motivation:**
  - Impurities segregate to GBs.



  - Enrichment of impurities at GBs -> cohesive properities of GB on macroscopic length scale.

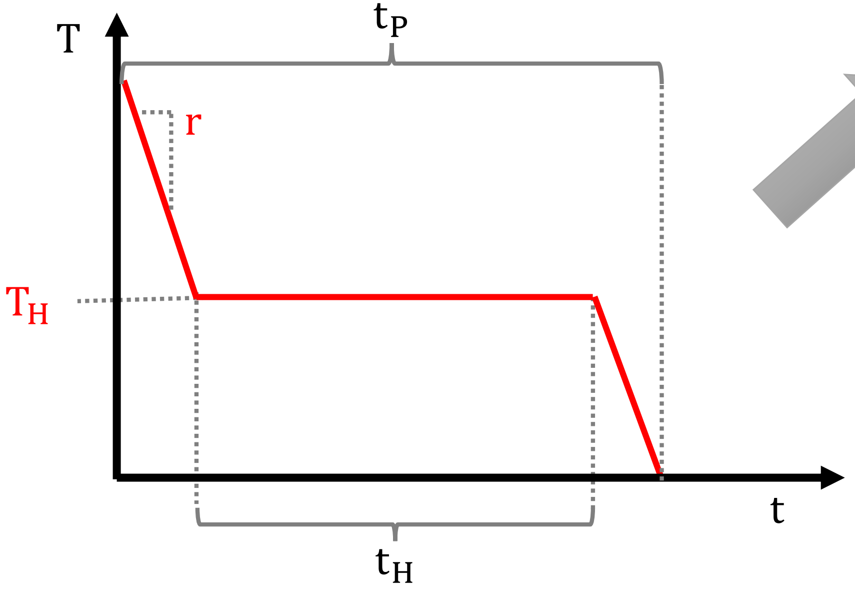


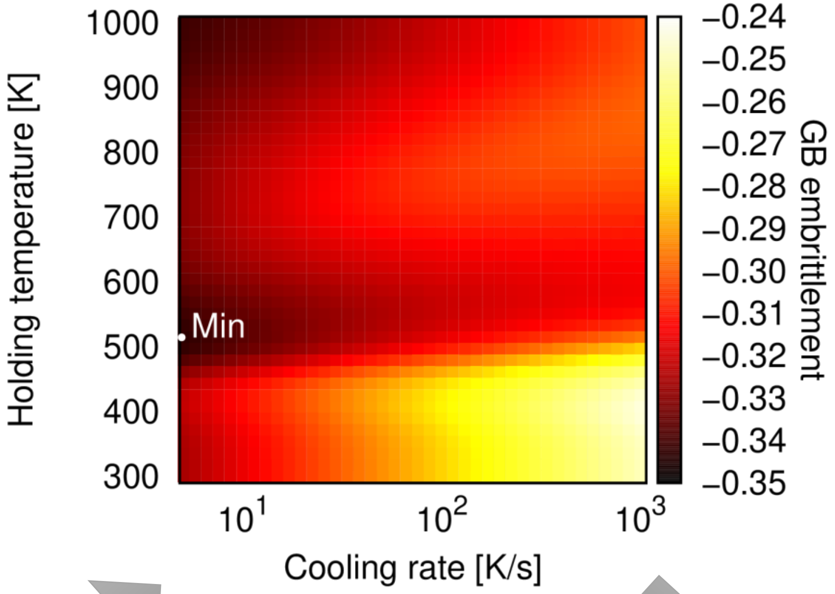
Daniel Scheiber and Lorenz Romaner

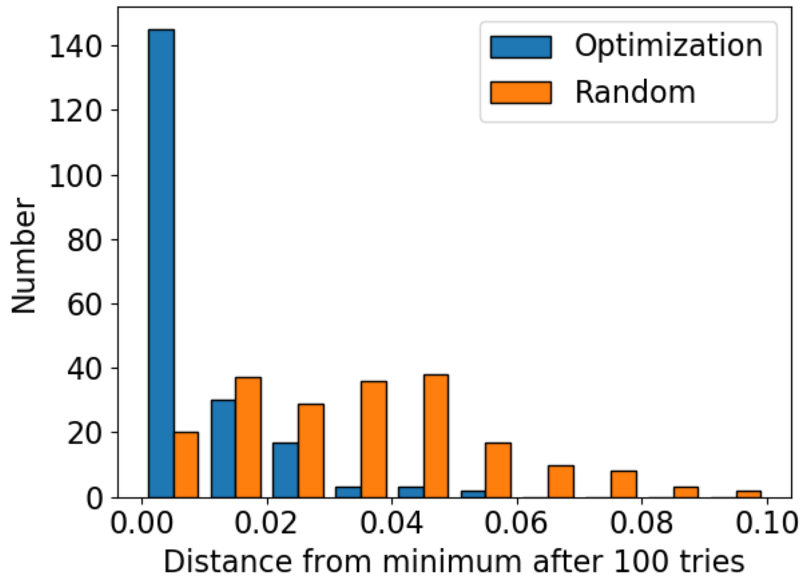
Features to optimize:

- **cooling rate**
- **holding temperature**

total process time is fixed to 1h







Use case: Solid solution strengthening

Franco Moitzi

High-throughput framework

Machine learning

Input: Alloy $\{c^{(n)}, c^{(n+1)}, \ldots, c^{(m)}\}$

Green's function DFT

Semiempirical E_{XC} correction

Finite temperature effects (phononic, magnetic, electronic)

C_{44}, C', B

$\frac{\partial V_{alloy}}{\partial c^{(n)}}$

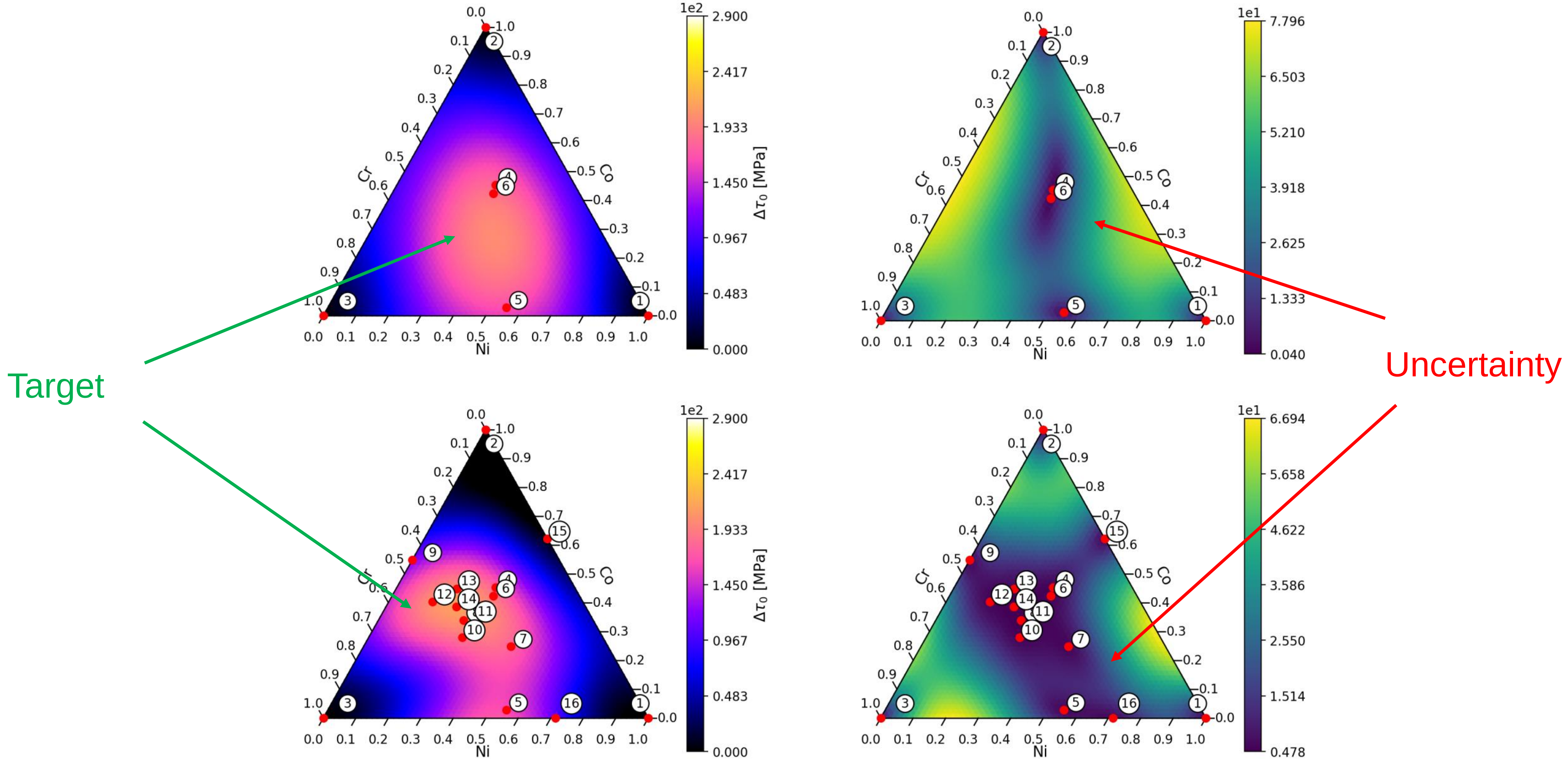
Strengthening model

$\Delta\tau = f(C_{44}, C', B, \frac{\partial V_{Alloy}}{\partial c_i}; T)$

Target quantity: $\Delta\tau_0$ Critical resolved shear stress

Workflow gives the critical resolved shear stress (CRSS) contribution due to solute solution strengthening

Franco Moitzi



- Adaptive learning is a universal approach to materials design
- Both experiment and ab initio data can be used on equal footing
- Lightweight techniques such as CPA (for alloys) and effective Hamiltonians (for perovskites) offer a lot of opportunities

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1) Veerapandiyan et a, submitted to Advanced Electronic Materials