

Theory-Guided Transformations of Inorganic Materials for Sustainable Energy Conversion and Storage

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(website)



Design of Materials on Computers

DMC LAB

Bartel Research Group

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01100 1 0 00 01101001
011 00 00 0110011
00100000 110 10 01111
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00100 0 01 0001 01101100
0110 0 01 00 1101110
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0110011 1 1 1 10100
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Teaching

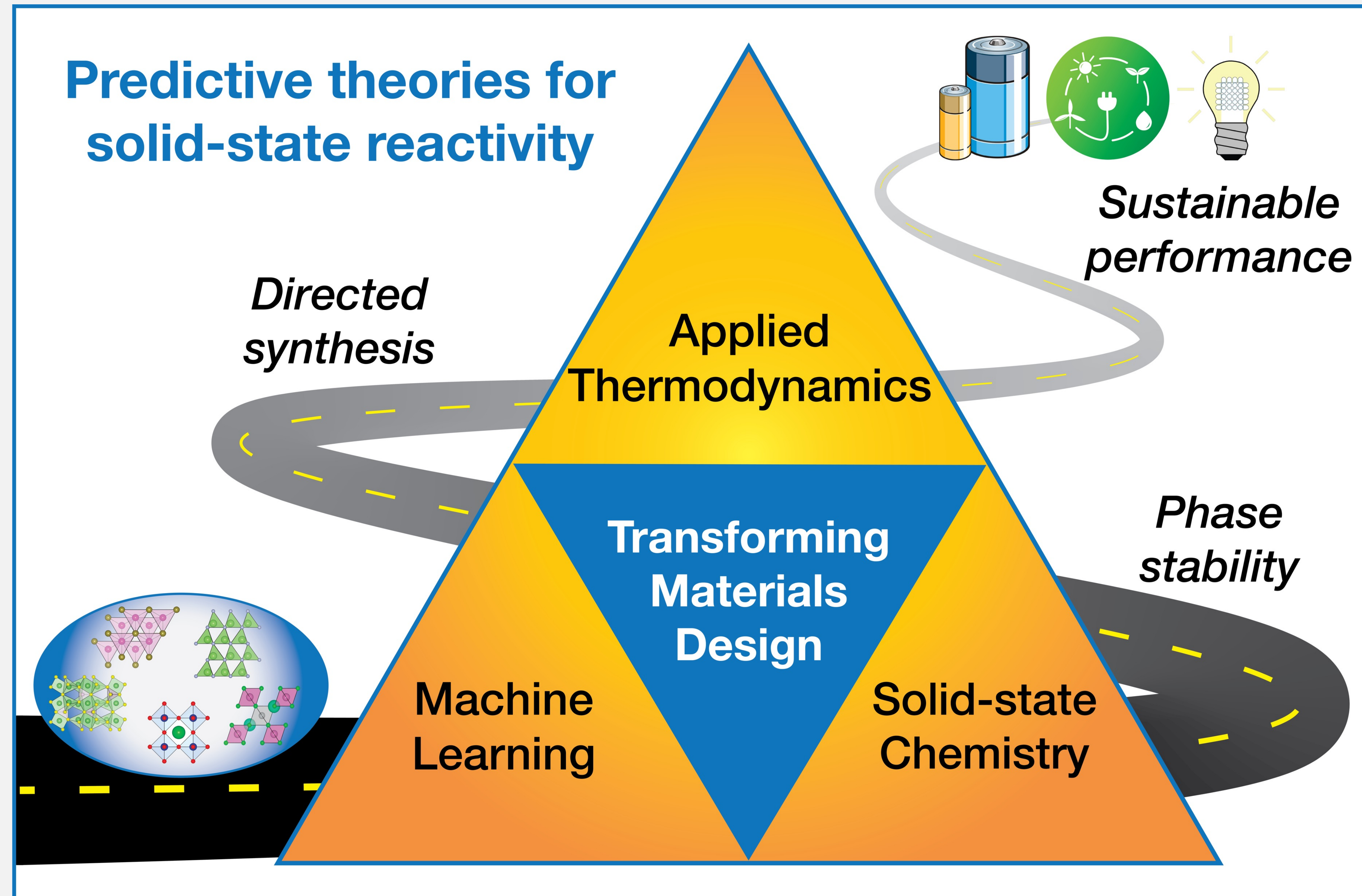
Thermodynamics $\Delta U = Q - W$
Data analysis $\hat{y} = X\beta + \epsilon$
Physical chemistry $\hat{H}\psi = E\psi$

Interactive Hands-on Engaging

FLIPPED
lecture classroom activities

Python, ML, nanoscale solids

$h\nu$ kT



Research highlights

Selected papers:
AM⁺, CJB⁺ et al., *Adv. Materials*, 2021, 33, 24
CJB⁺ et al., *npj Computational Materials*, 2020, 6 (97)
CJB⁺ et al., *JACS*, 2020, 142 (11) 5135
CJB⁺ et al., *Science Advances*, 2019, 5, eaav0693
WS, CJB et al., *Nature Materials*, 2019, 18, 732
CJB et al., *Nature Communications*, 2018, 9, 4168

Core skills

Computational chemistry

ASP, LOBSTER, MATERIALS PROJECT

Materials design

Phase diagrams, crystal structures

Data science

Bayesian inference, neural networks

Materials synthesis by design

hydrothermal, precipitation, ceramic

μ , Φ , P , T , pH, γ

What conditions stabilize metastable materials and why?

Principles for the design of reversible redox materials

reduction, oxidation, solar fuels, rechargeable batteries

DOS, COHP, ELF

templated polymorph

topotaxy (ion exchange), epitaxy (film growth)

Leverage descriptors for kinetic control in materials synthesis

Machine learning to explore materials space

1. Which compositions?
2. Which structures?
3. Where to supplement data?

$\hat{H}\psi = E\psi$