



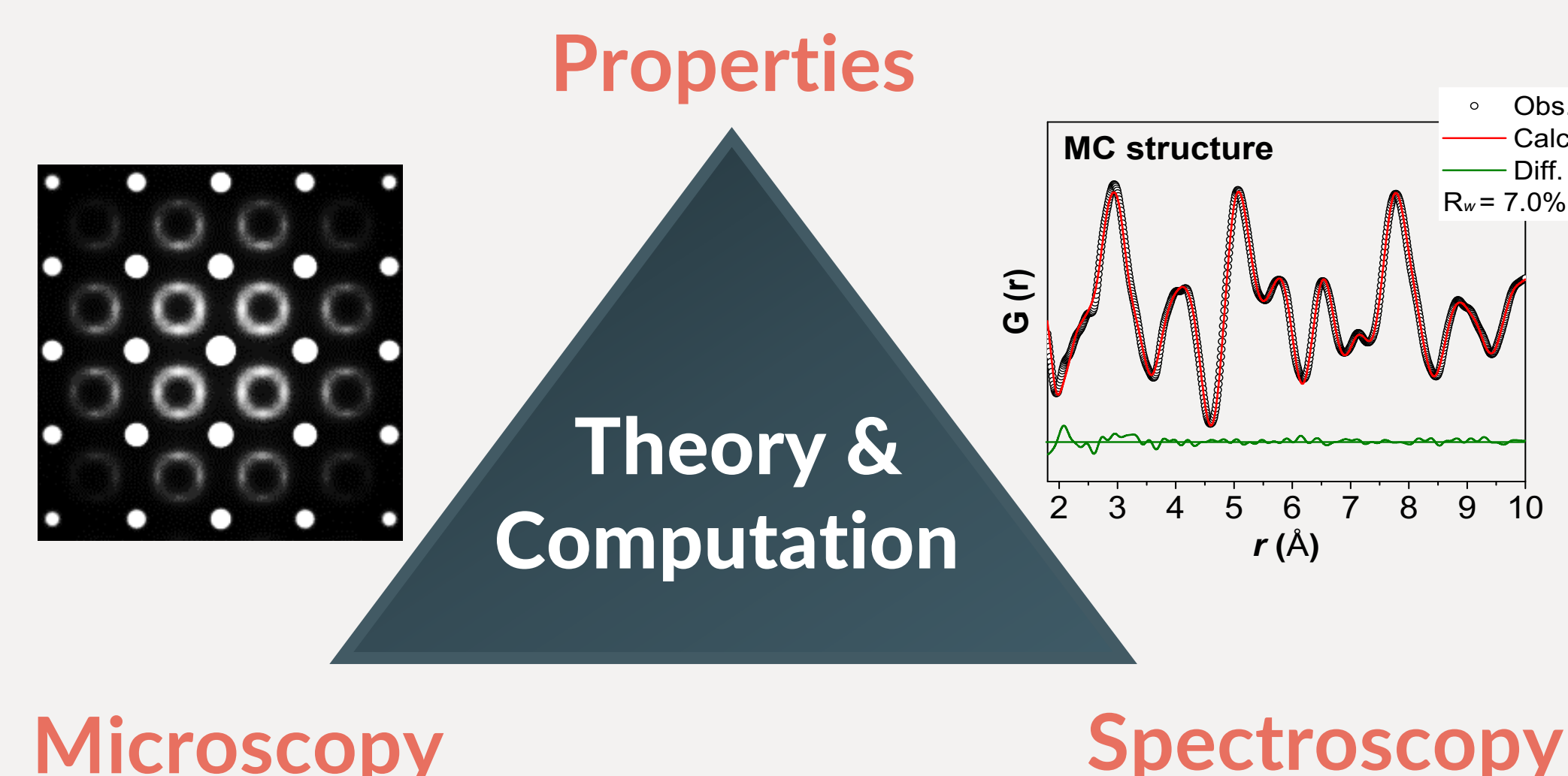
# Dr. Bin Ouyang's Research Group (We are hiring!)

## Data science solution to energy storage and conversion

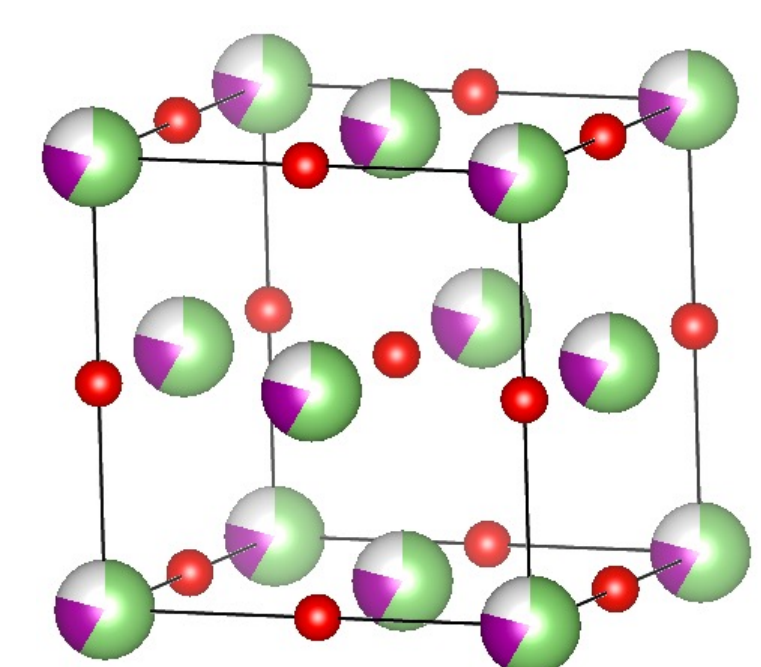
Email: [bouyang@fsu.edu](mailto:bouyang@fsu.edu)

Area: Computational Chemistry, Environment and Energy, Solid State Chemistry, Synthesis and Catalysis

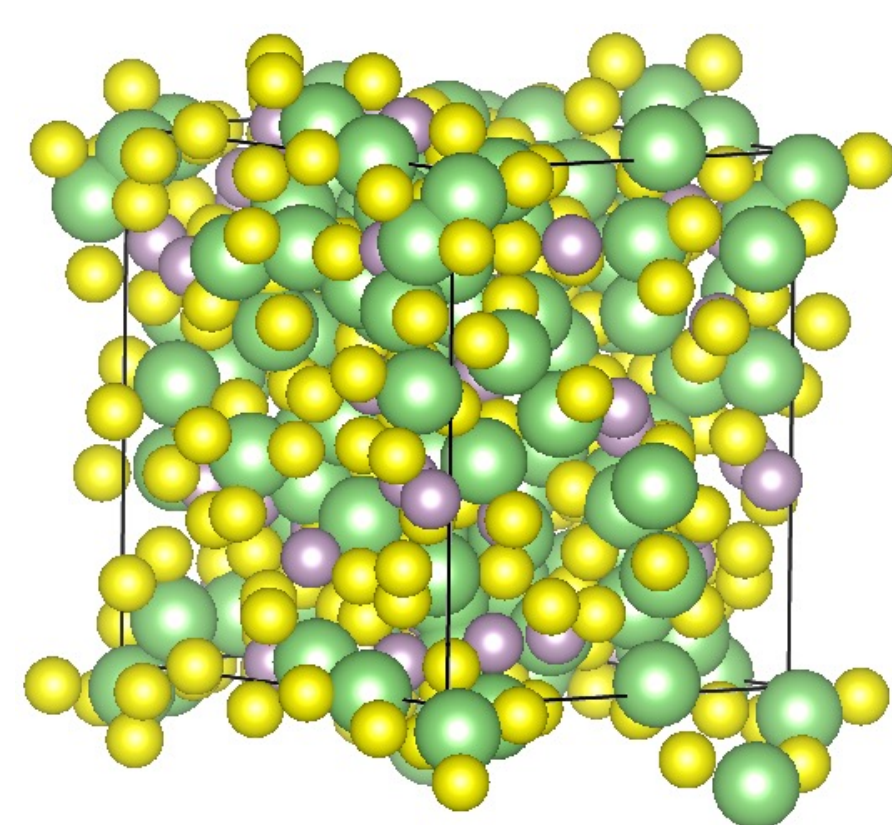
### Local structure–property relationship



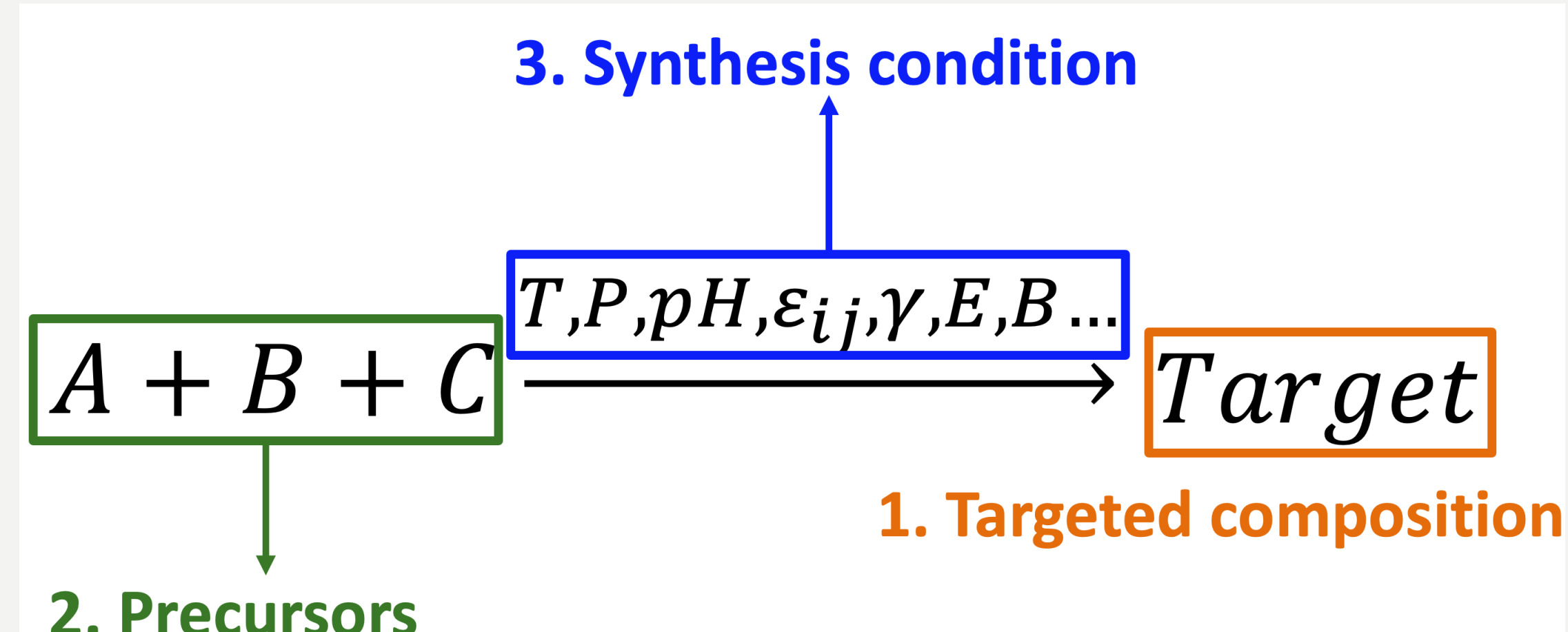
### Compositional disorder



### Structural disorder

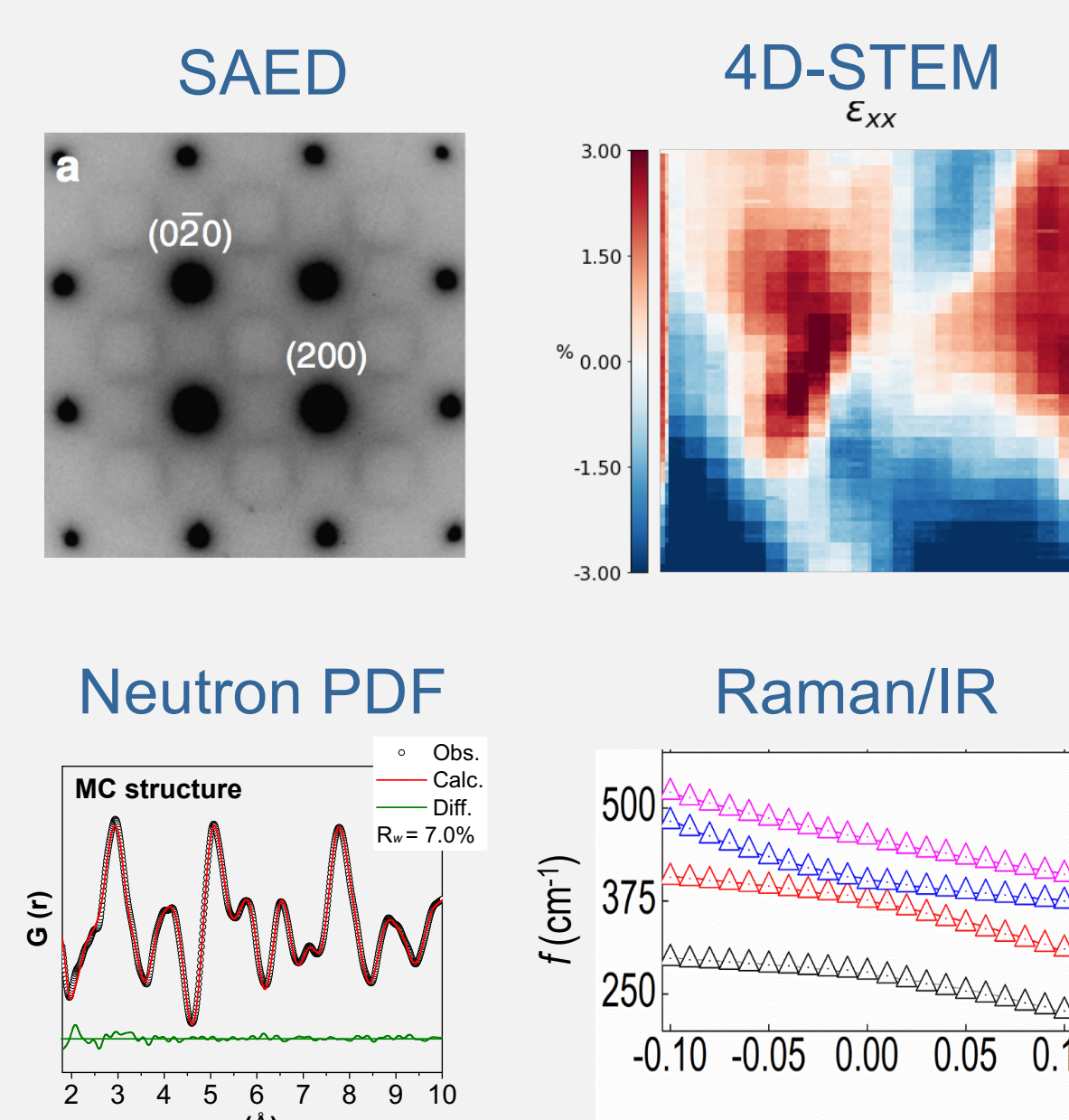


### Predictive synthesis



### Characterization featured dataset

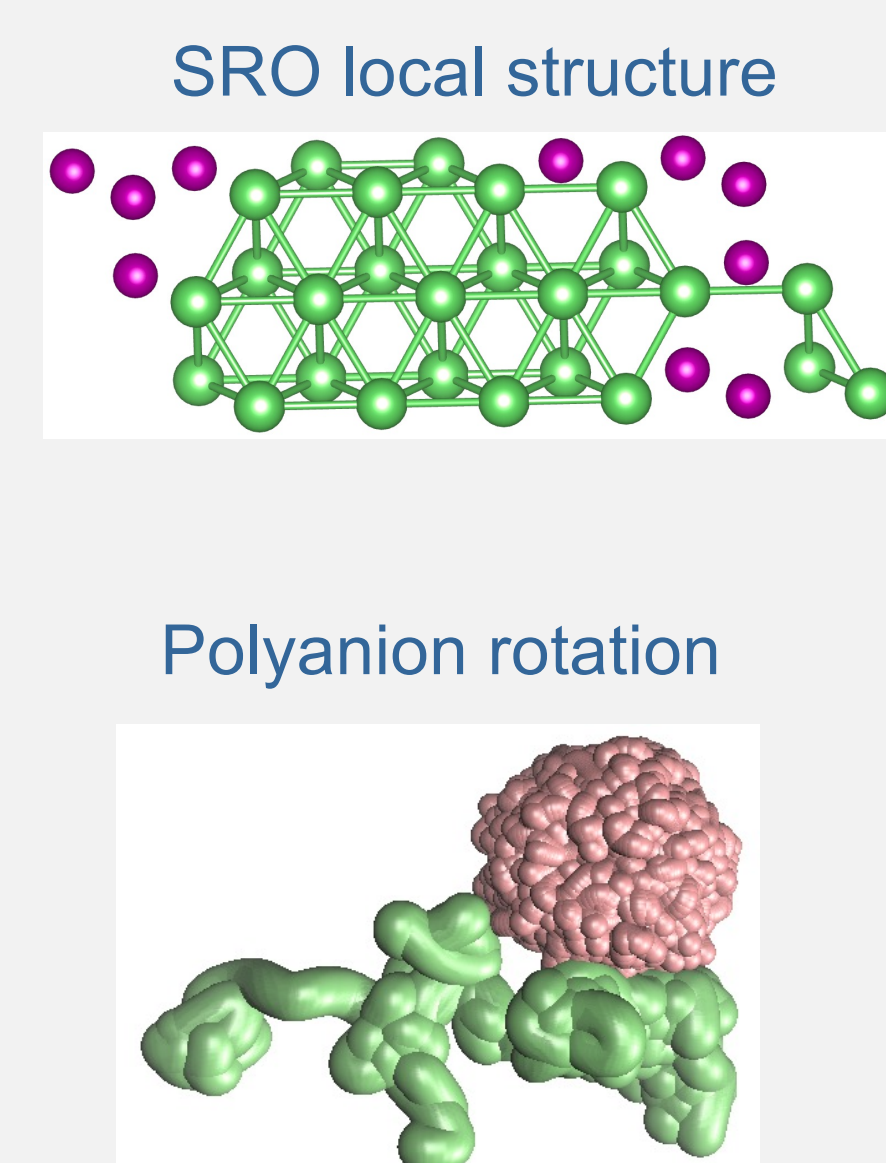
- Text/image mining
- Literature
- Collaboration



• Nature Materials, 20, 214–221, 2021

### Computational-aided reconstruction

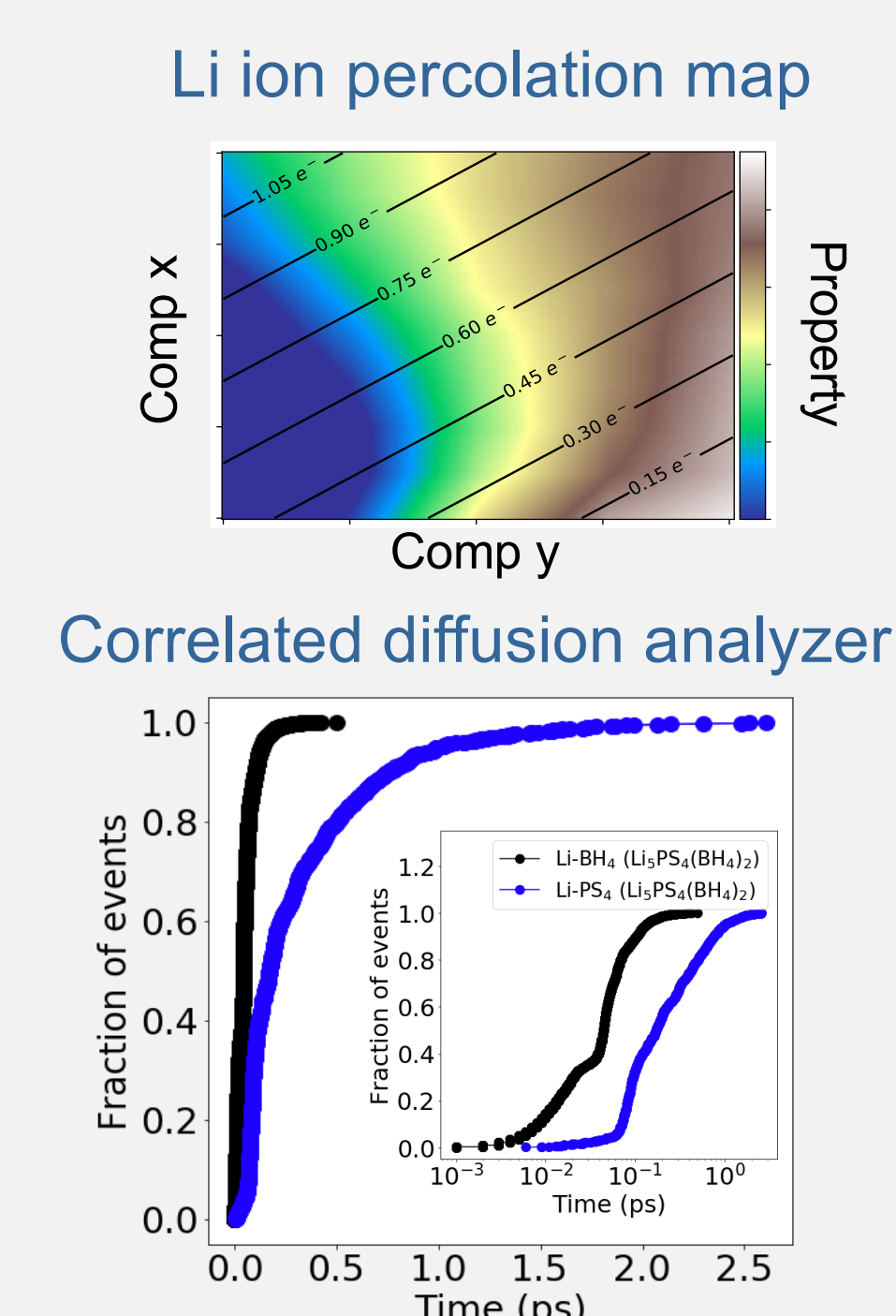
- Multiscale physical model
- Computer vision
- Machine learning



• Advanced Energy Materials, 10, 1903240, 2020

### Local structure–property mapping

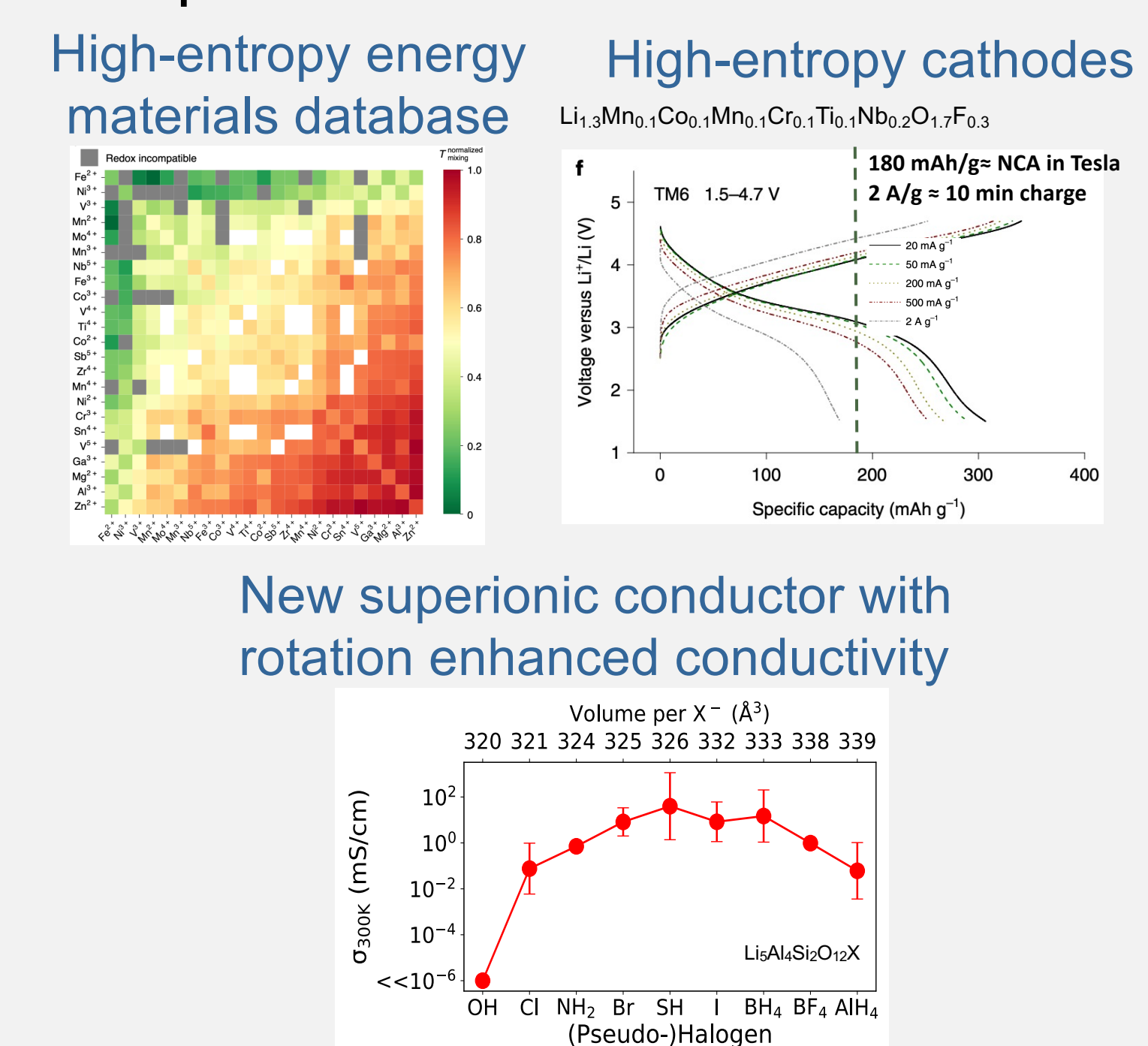
- Ionic diffusion
- Electronic structure
- Interface and surface



• Chem 6, 153–168, 2020

### Local structure-driven materials prediction

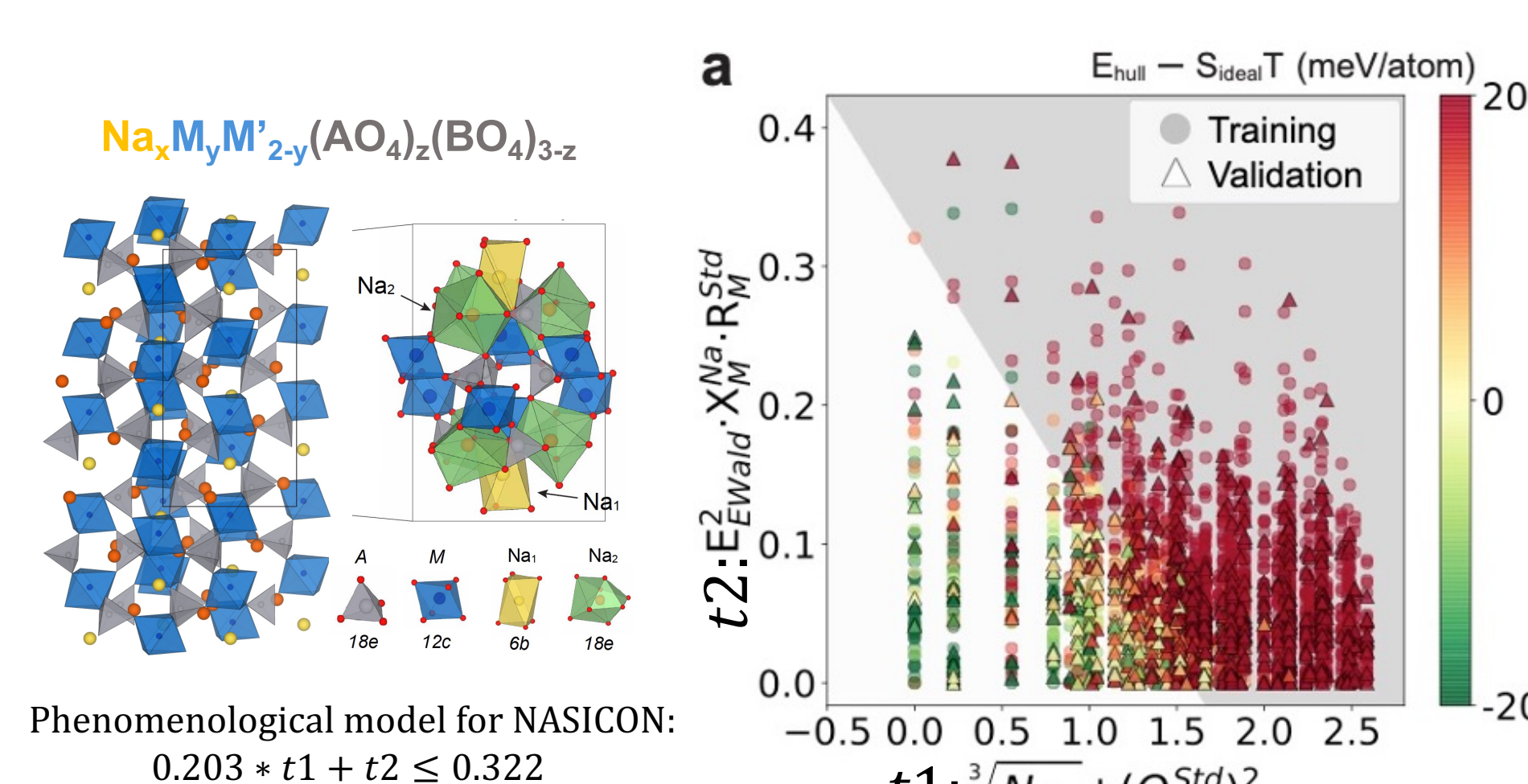
- High throughput screening
- Theoretical prediction
- Experimentation



• Nature Materials, 20, 214–221, 2021

### Targeted composition

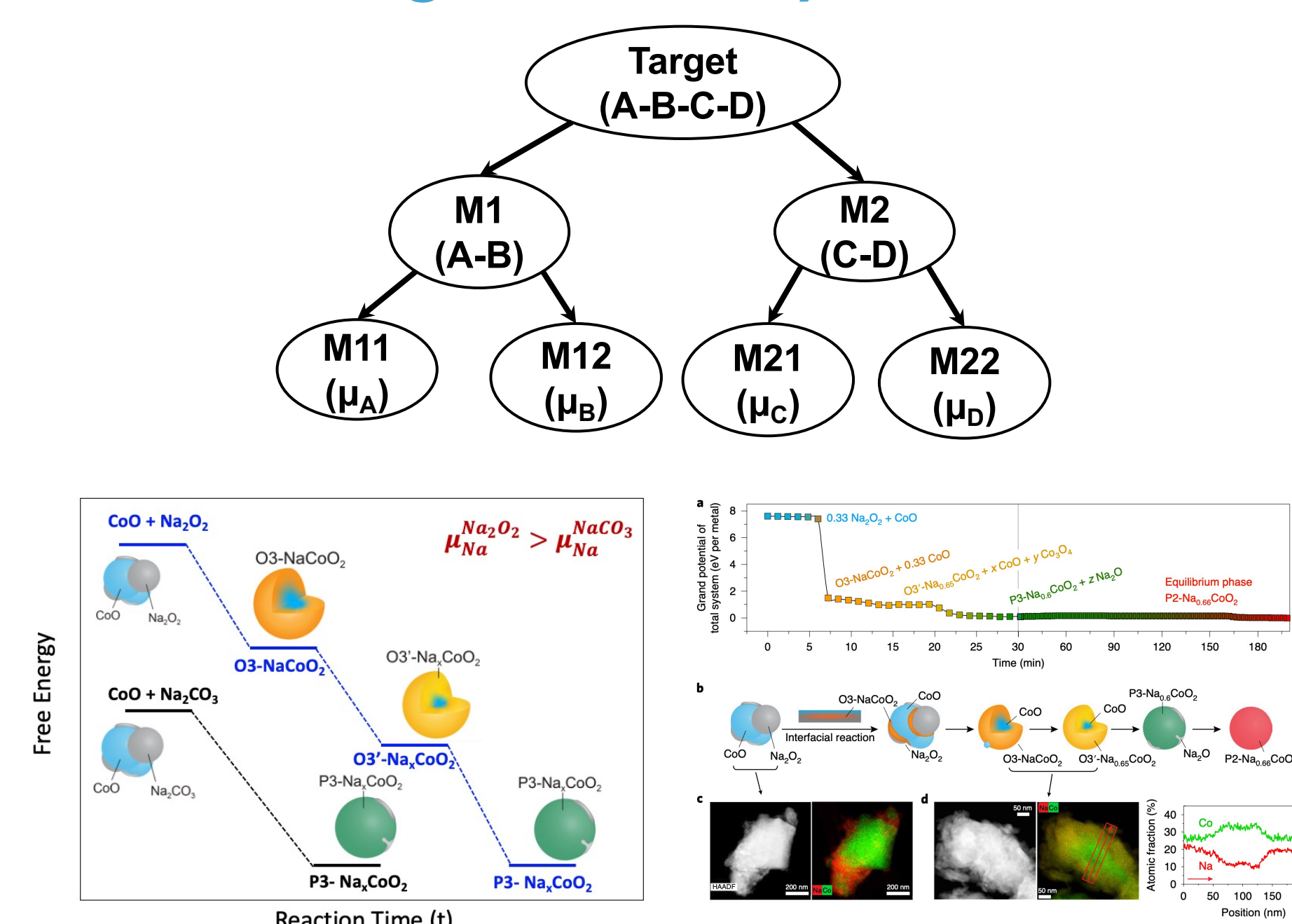
#### Machine-learnt phenomenological model



• Nature Communications, 12, 5752, 2021

### Feasible precursors

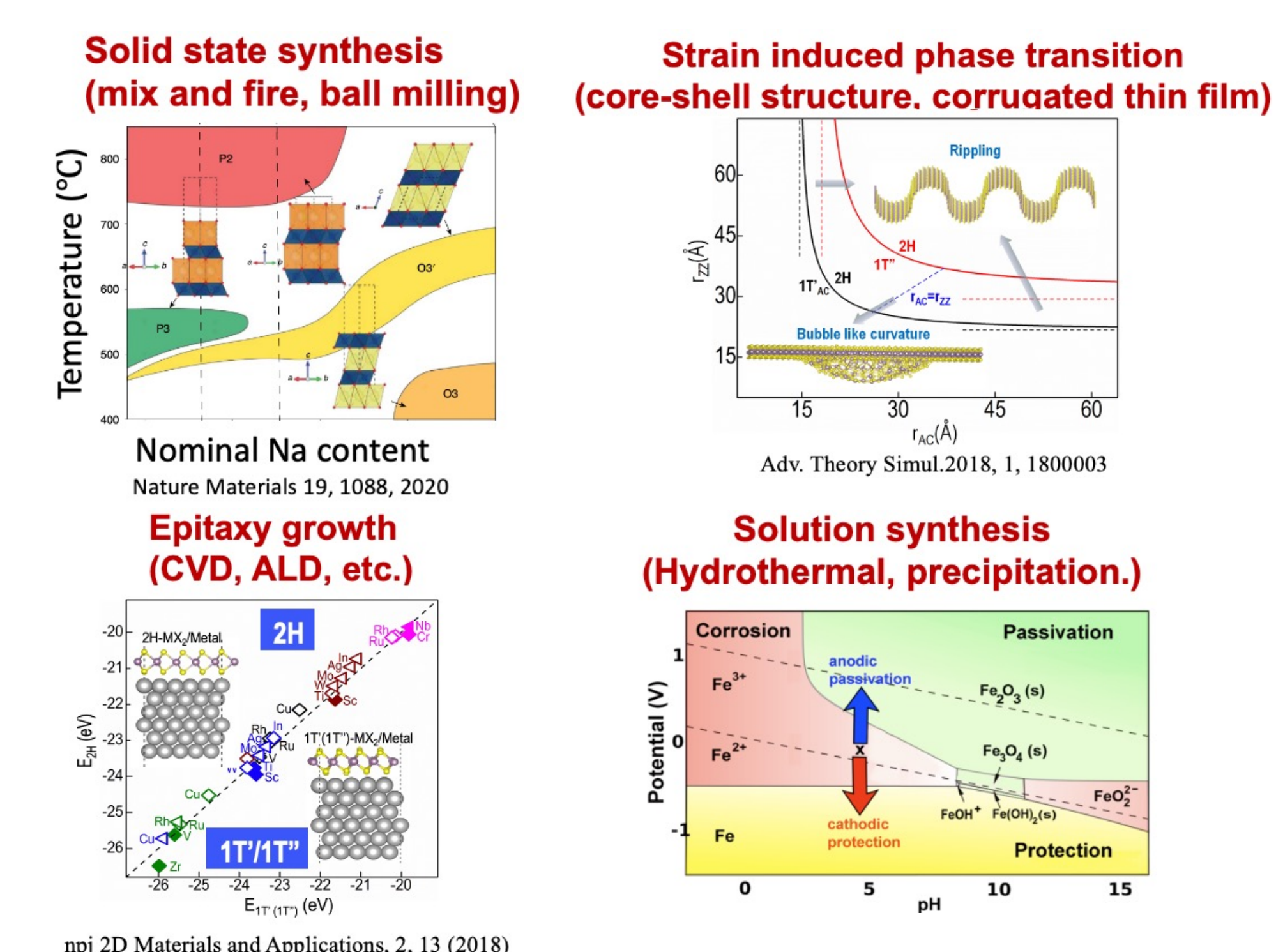
#### Inorganic retrosynthesis



• Nature Materials, 19, 1088–1095, 2020

### Accessible synthesis conditions

#### Synthesis/rudimentary phase diagrams



### Things you can learn:

- Quantum chemistry calculations
- High throughput computation
- Data mining and machine learning
- Database and web development
- Thermodynamics and kinetics
- Percolation theory
- More.....

### Resources provided

- Regular access to most powerful computer in campus: Research Computer Center
- Access to most powerful supercomputers in United states: NERSC, XSEDE, Eagle, etc.
- In-house high performance workstations: GPU workstations and CPU workstations
- Your advisor's passion, insight and instruction on materials informatics 😊

LinkedIn

Google Scholar

My Website

