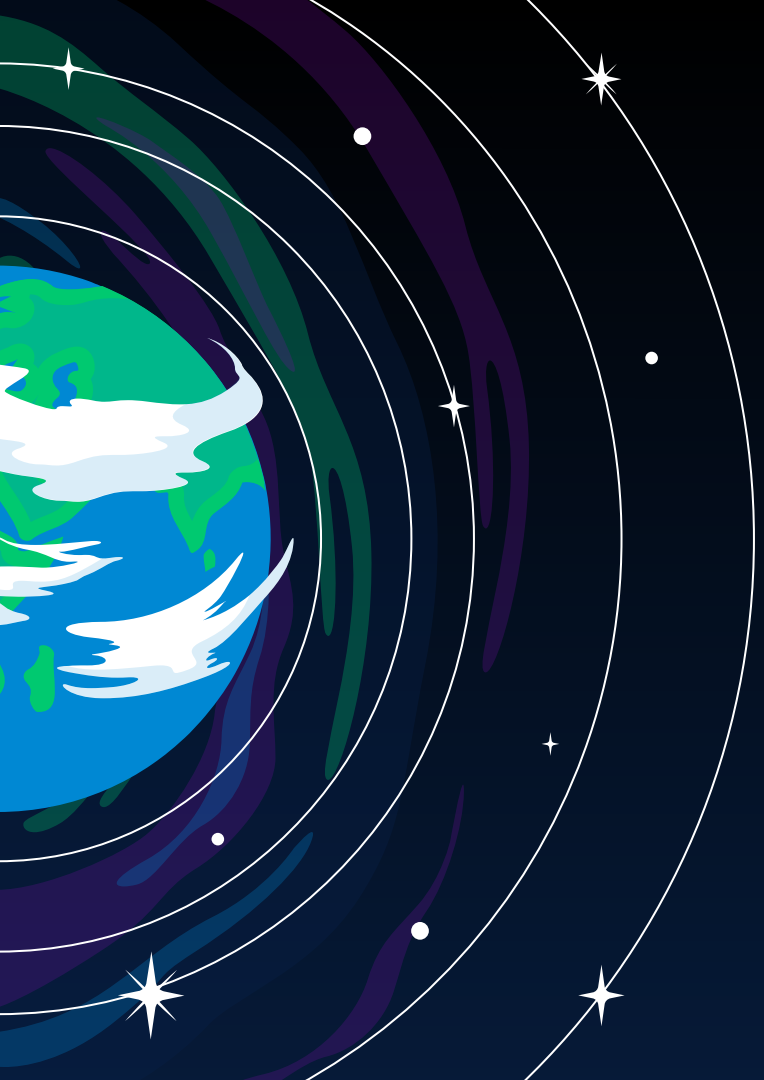


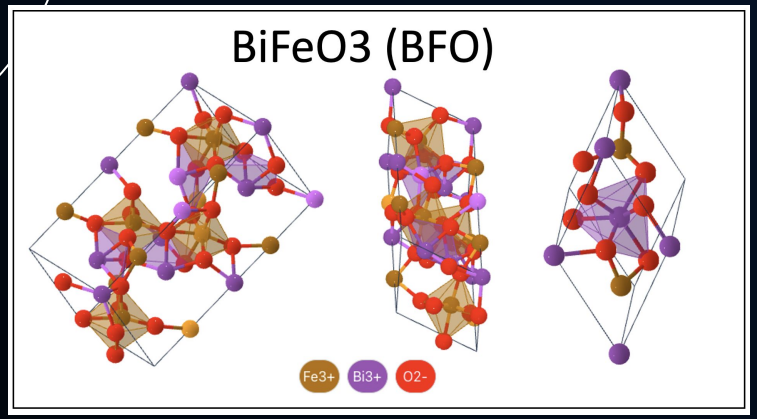
BERKELEY LAB

Precursor Reaction Pathway Leading to BiFeO3 Formation: Insights from Text-Mining and Chemical Reaction Network

Viktoriia Baibakova
PhD candidate at UC Berkeley

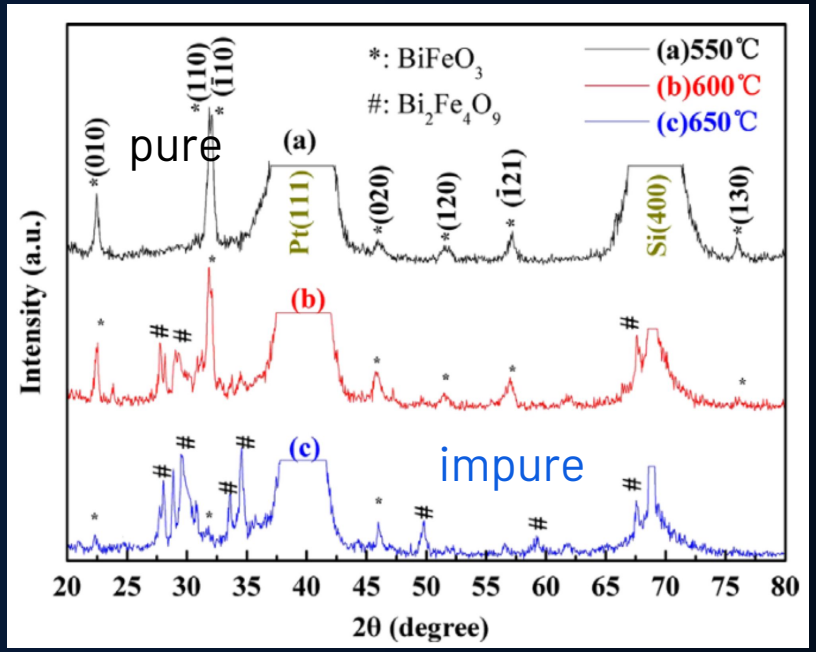
2024 NASA Aerospace Battery Workshop
Huntsville, AL, USA

BiFeO3 Perovskite Thin Films

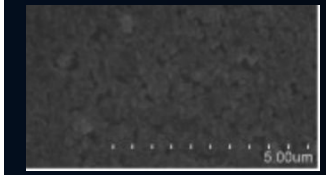


- Perovskite
- Multiferroic
- Non-toxic
- Phase-pure

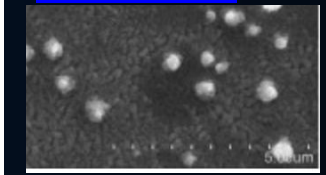
Impurities degrade electric, Ferroelectric, and PV response

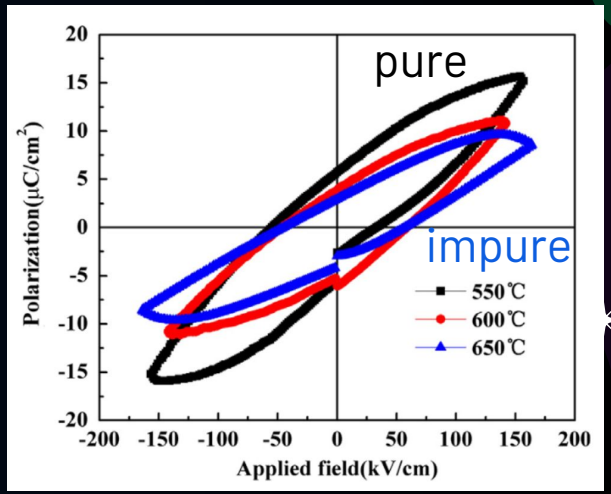


Phase-pure BiFeO3



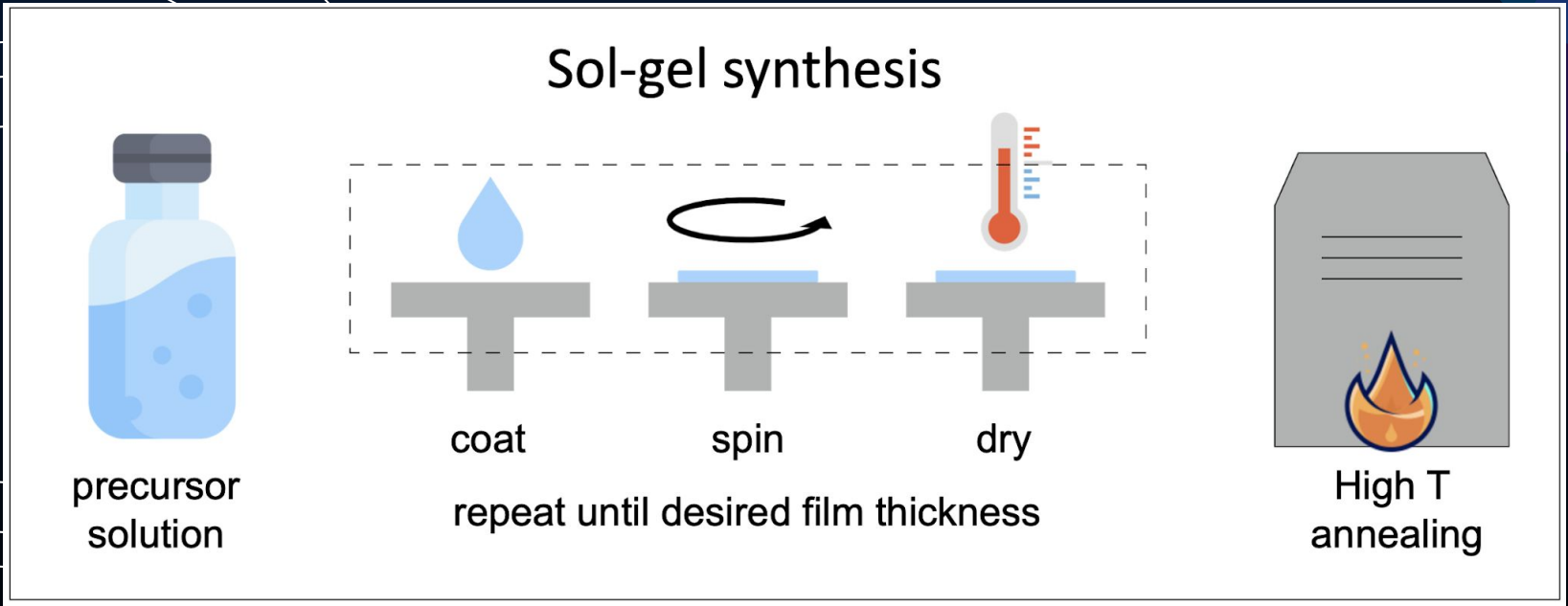
BiFeO3 + Bi2Fe4O9





Biswas, P. P., et al. "Dipole pinning effect on photovoltaic characteristics of ferroelectric BiFeO3 films." *Journal of Applied Physics* 123.2 (2018).

Sol Gel Synthesis



Method

a.

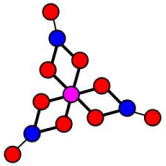
Text-Mining

DOI	Bi & Fe salts	Solvent	...	Crystallinity
10.1007/...28-3	Nitrates	2-methoxyethanol	...	Phase-pure
10.1007/...61-9	Nitrates	ethylene glycol	...	Bi2Fe4O9

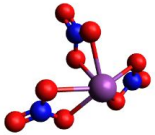
b.

Chemical Reaction Network

1. Produce graphs of species



2. Generate 3D representations



3. Optimize, calculate energy

QuAcc

Q-CHEM

Dataset of species

4. Build CRN

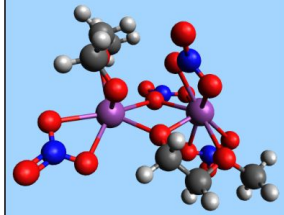
HiPRGen

5. Analyze reaction pathway

RNMC

c.

Path: Dimerization



Energetically favorable

Seeds phase structure

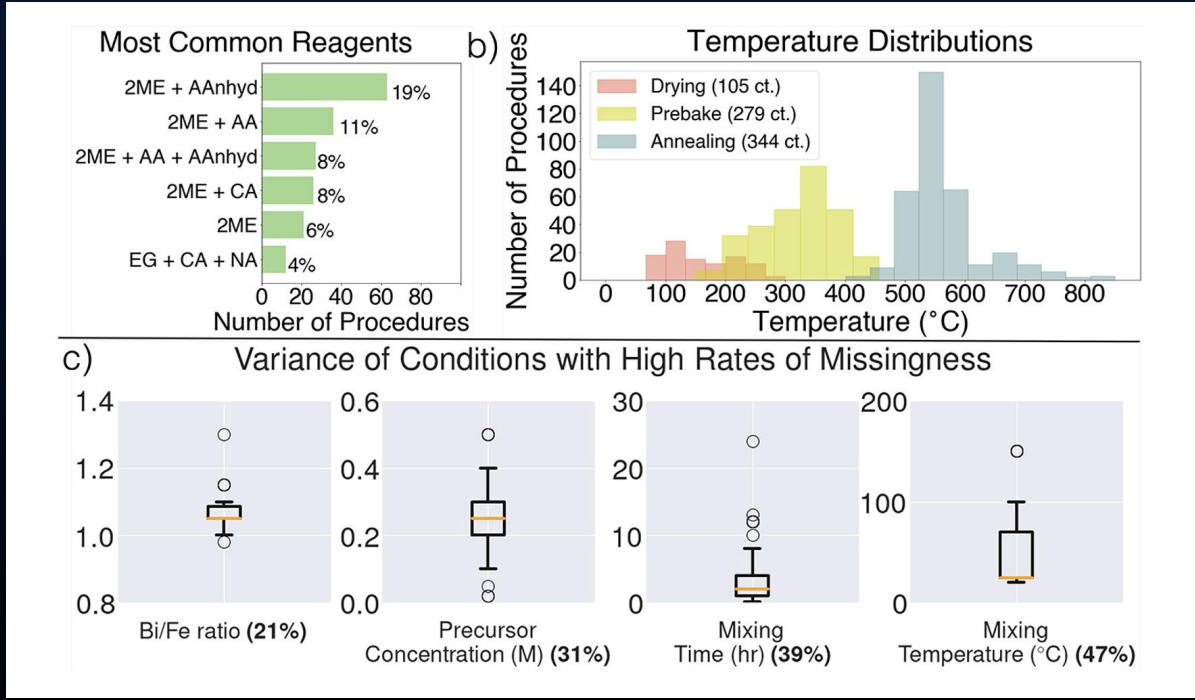
Promoted:
- nitrates
- solvents*

Inhibited:
- surfactants

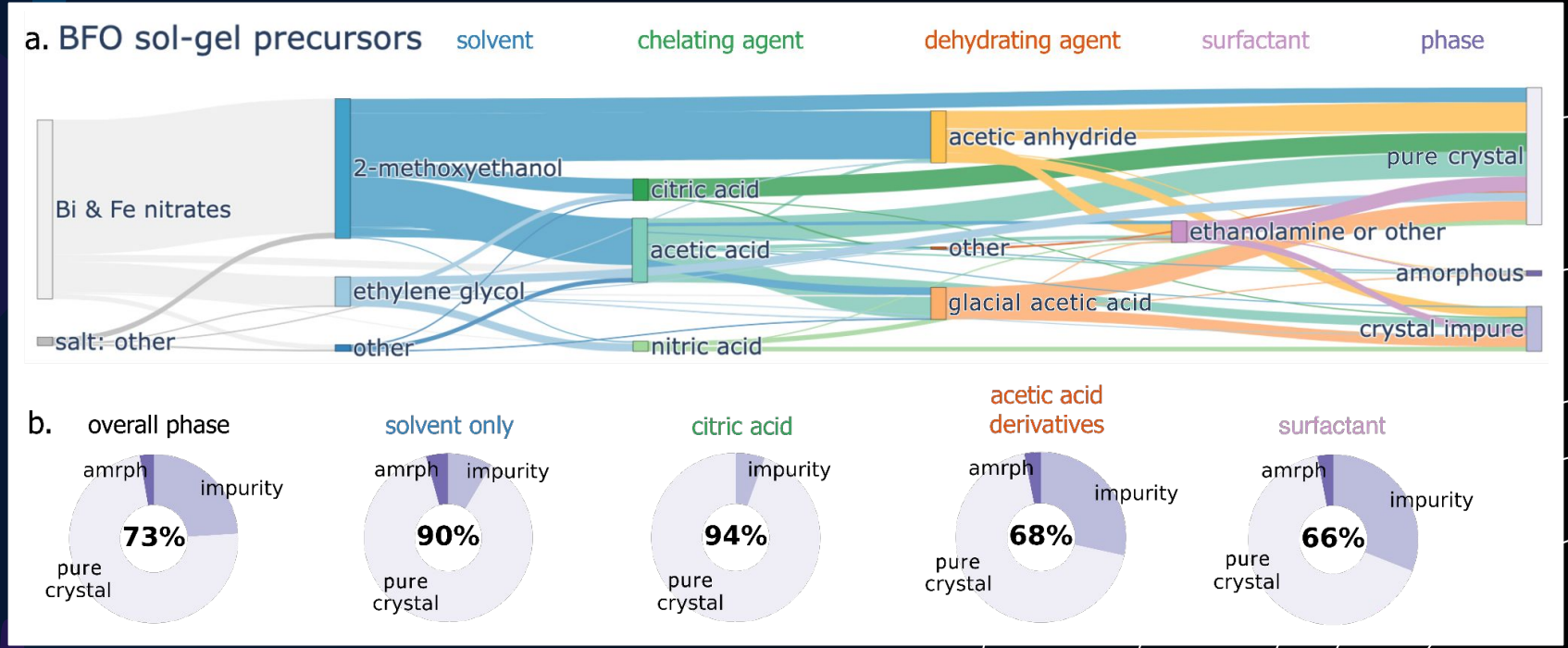
01

Text Mining

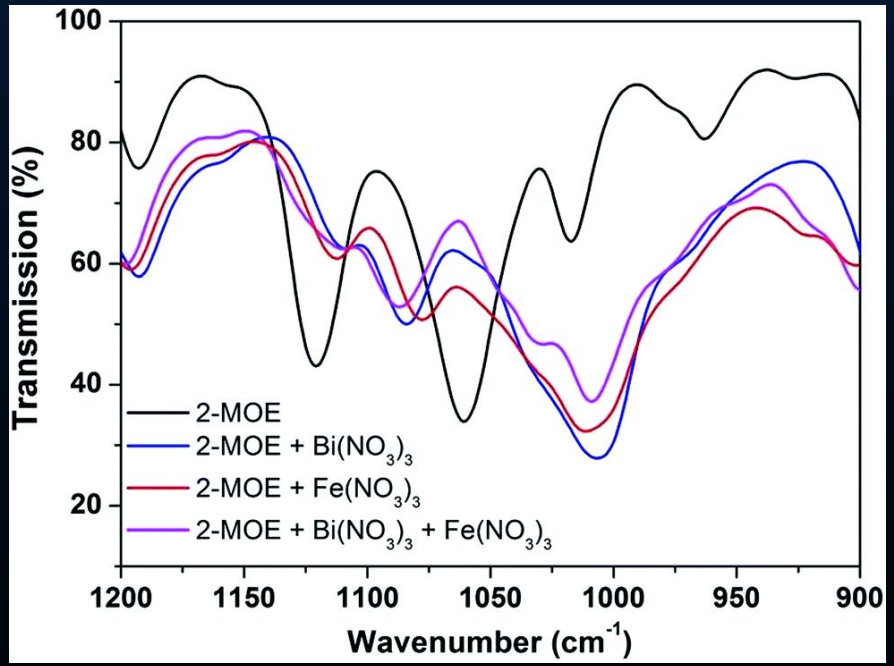
Data Analysis of Syntheses Mined from Text



Data Analysis of Syntheses Mined from Text



System for Reaction Pathway Analysis



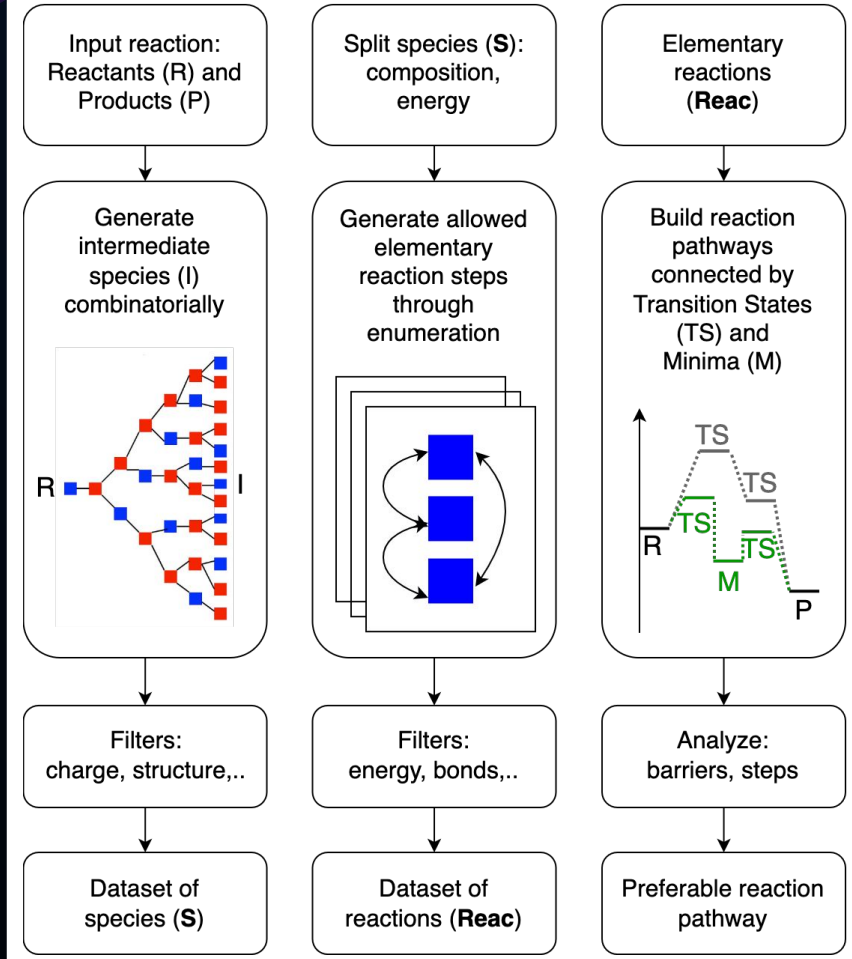
- Bismuth nitrate salt [Bi(NO3)3]
- 2-methoxyethanol solvent 2ME, 2MOE

Zhang, Qi, Nagarajan Valanoor, and Owen Standard. "Epitaxial () BiFeO3 thin-films with excellent ferroelectric p001roperties by chemical solution deposition-the role of gelation." *Journal of Materials Chemistry C* 3.3 (2015): 582-595.

02

Chemical Reaction Network

Chemical Reaction Network



Method

a.

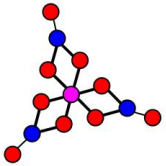
Text-Mining

DOI	Bi & Fe salts	Solvent	...	Crystallinity
10.1007/...28-3	Nitrates	2-methoxyethanol	...	Phase-pure
10.1007/...61-9	Nitrates	ethylene glycol	...	Bi2Fe4O9

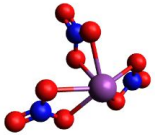
b.

Chemical Reaction Network

1. Produce graphs of species



2. Generate 3D representations



3. Optimize, calculate energy

QuAcc

Q-CHEM

Dataset of species

4. Build CRN

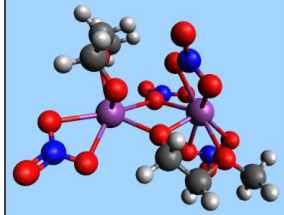
HiPRGen

5. Analyze reaction pathway

RNMC

c.

Path: Dimerization



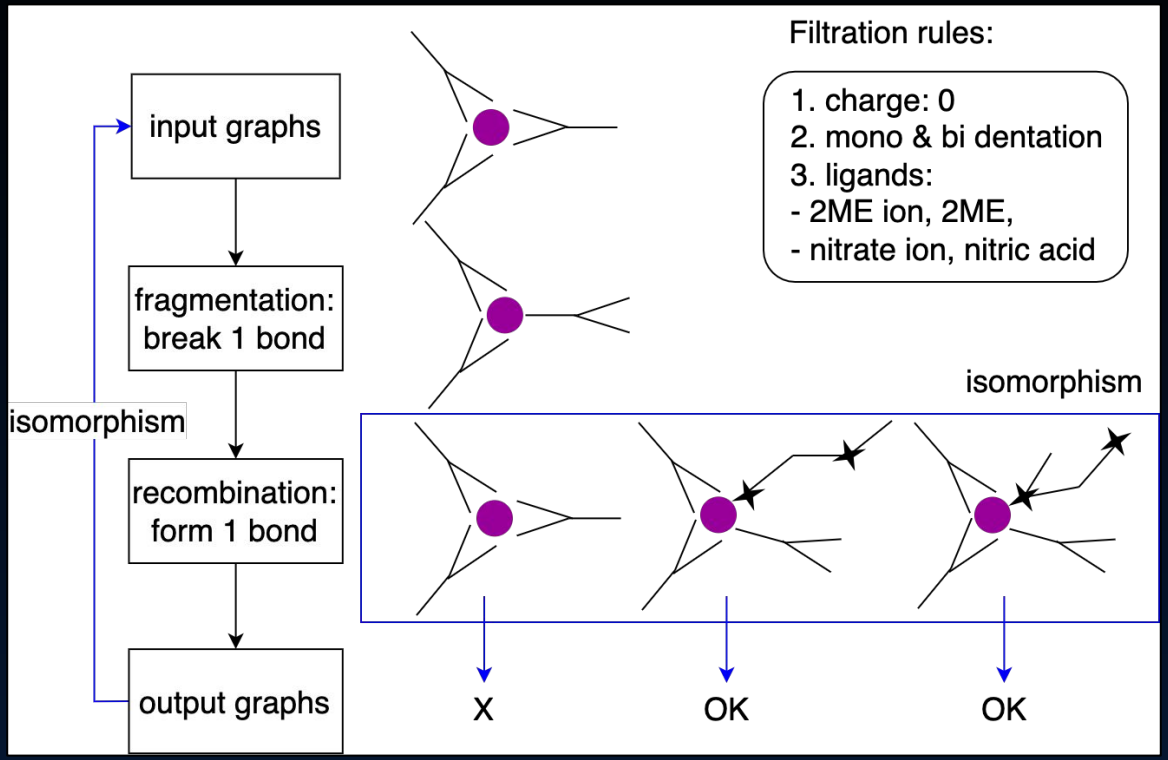
Energetically favorable

Seeds phase structure

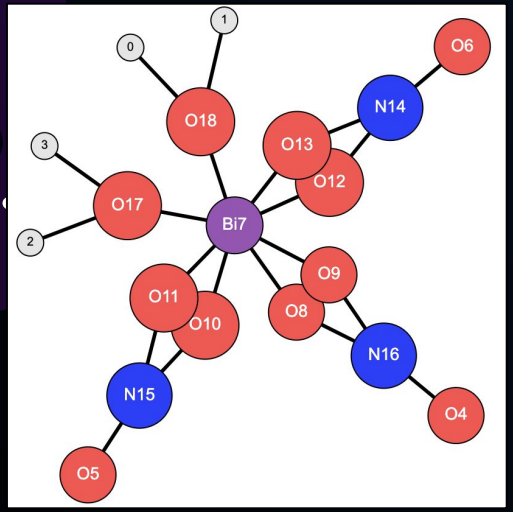
Promoted:
- nitrates
- solvents*

Inhibited:
- surfactants

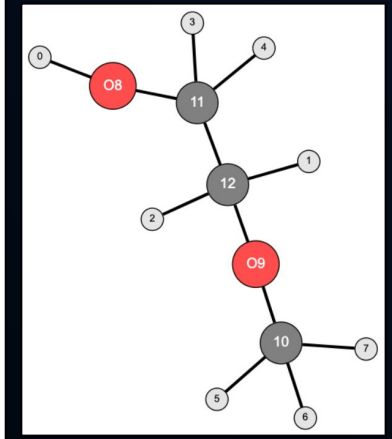
Intermediates Generation



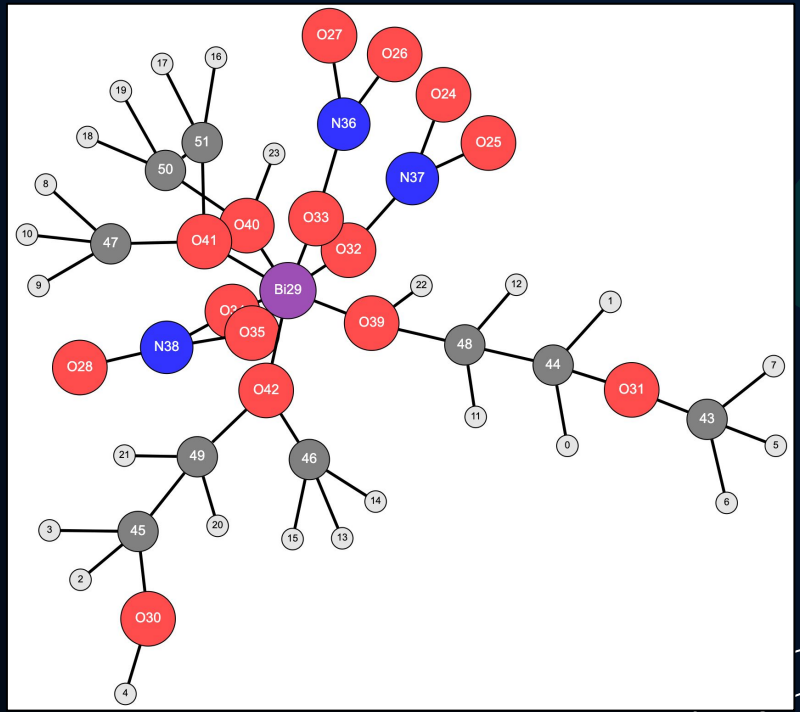
Molecular Graphs



Bi nitrate

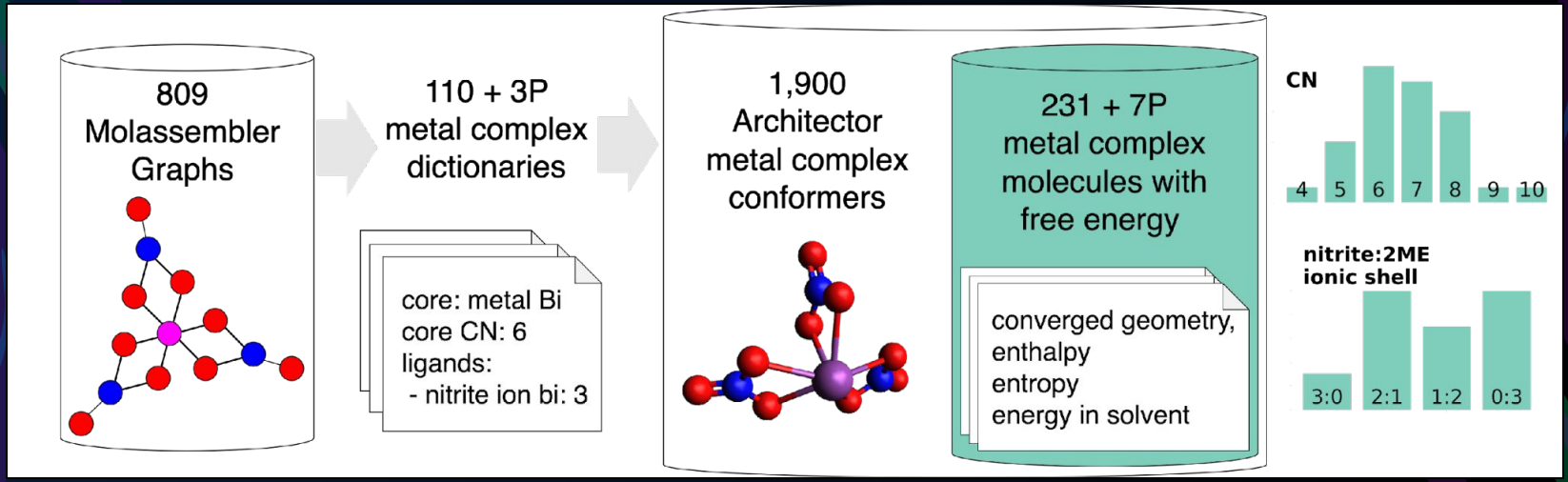


Solvent
2MOE

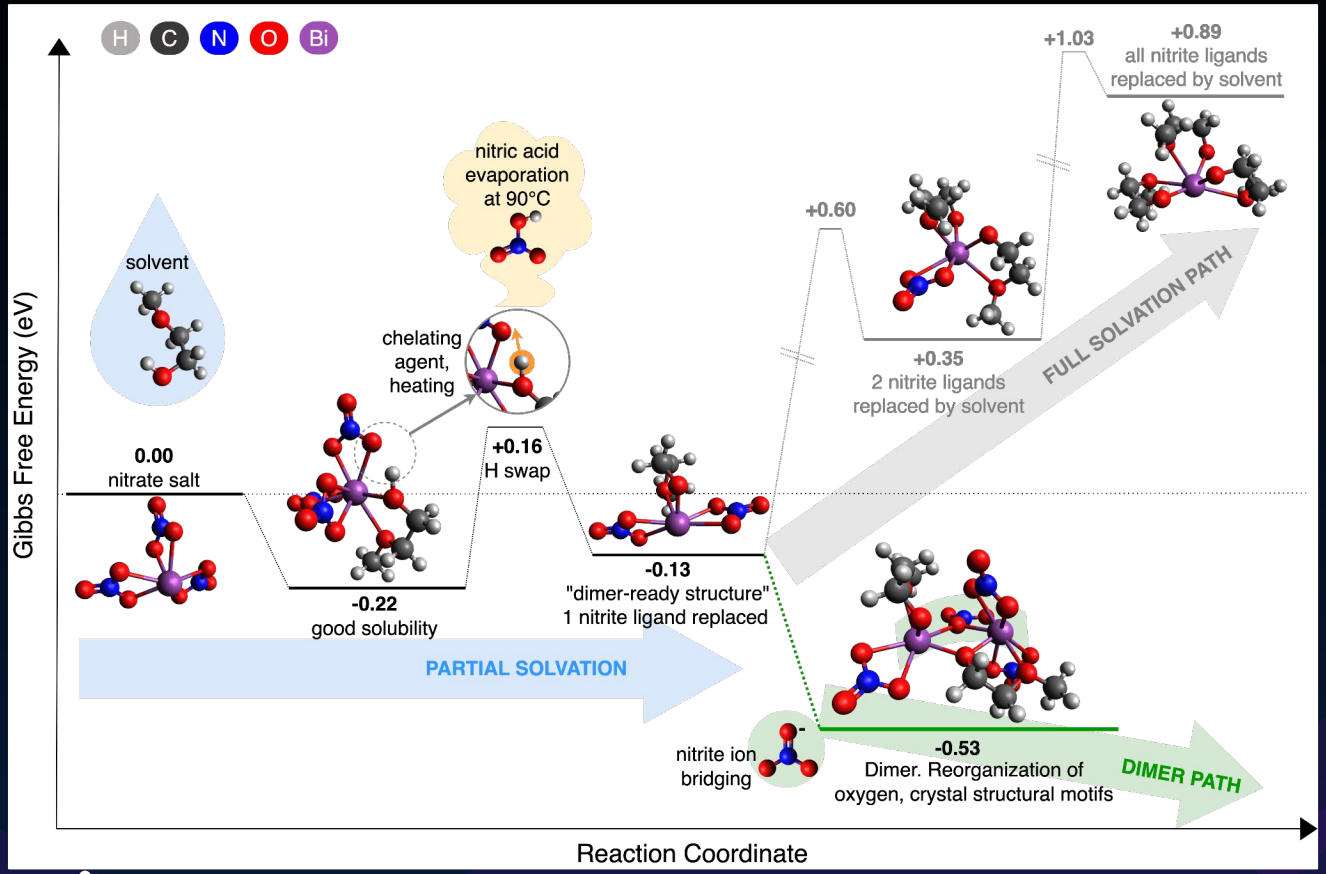


Intermediate specie

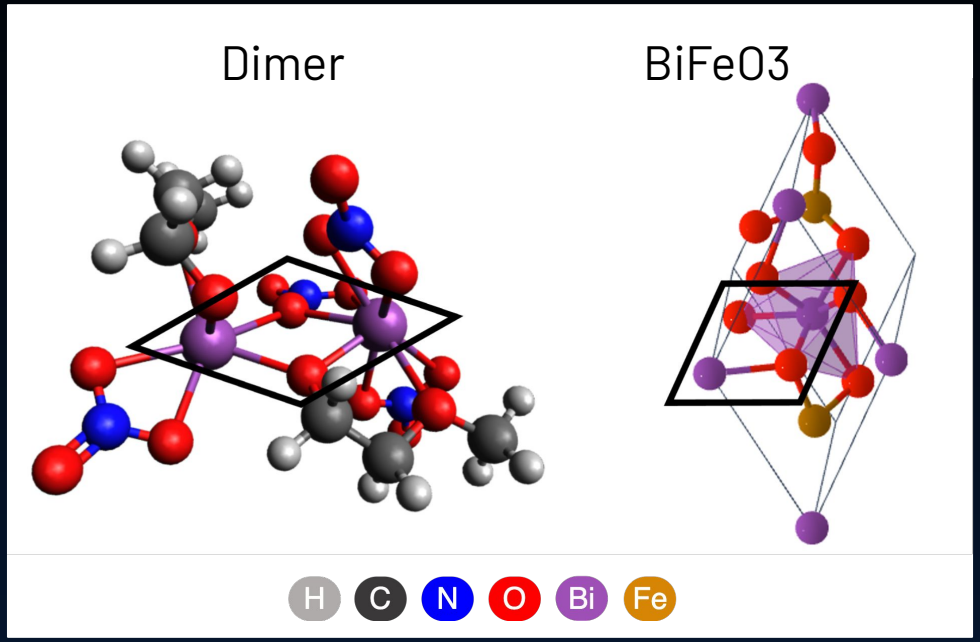
Dataset


809
Molassembler
Graphs
110 + 3P
metal complex
dictionaries
core: metal Bi
core CN: 6
ligands:
- nitrite ion bi: 3
1,900
Architector
metal complex
conformers
231 + 7P
metal complex
molecules with
free energy
converged geometry,
enthalpy
entropy
energy in solvent
CN
4
5
6
7
8
9
10
nitrite:2ME
ionic shell
3:0
2:1
1:2
0:3

Dimerization is Preferable Pathway



Rhombohedral Structural Motifs



Conclusions

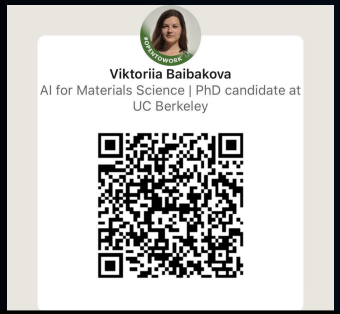
- Text-mining analysis of 340 synthesis recipes for phase-pure BFO
- Additives lead to variable crystallinity
- CRN: dimer route is preferential
- Dimer sets the structural motifs of the resultant BFO phase
- Dimer-related works: surfactant obstructs oligomerization
- Dimer-related works: solvent stabilizes de-nitrated complex

Conclusion: text-mining motivated system for CRN → CRN revealed true mechanism → related works elaborated text-mining results

Preprint: 10.26434/chemrxiv-2024-xj01h

THANKS!

Let's connect!



FUNDING:

CHiPPS Center for High Precision Patterning Science

NERSC

Los Alamos NATIONAL LABORATORY

BERKELEY LAB

CREDITS: This presentation template was created by **Slidesgo**, including icons by **Flaticon**, and infographics & images by **Freepik**

TEAM:

Dr. **Kevin Cruse**, LBNL

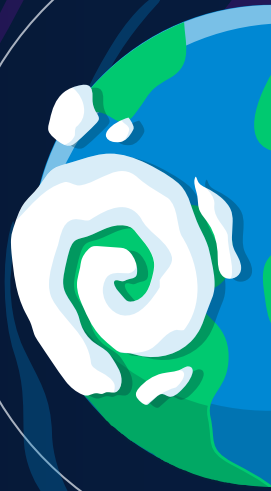
Dr. **Michael G. Taylor**, LANL

Dr. **Carolin M. Sutter-Fella**, LBNL

Prof. **Gerbrand Ceder**, LBNL

Lead PI
Dr. **Anubhav Jain**, LBNL

Lead PI
Dr. **Samuel M. Blau**, LBNL



This trip was supported by **The Graduate Division,** University of California at Berkeley