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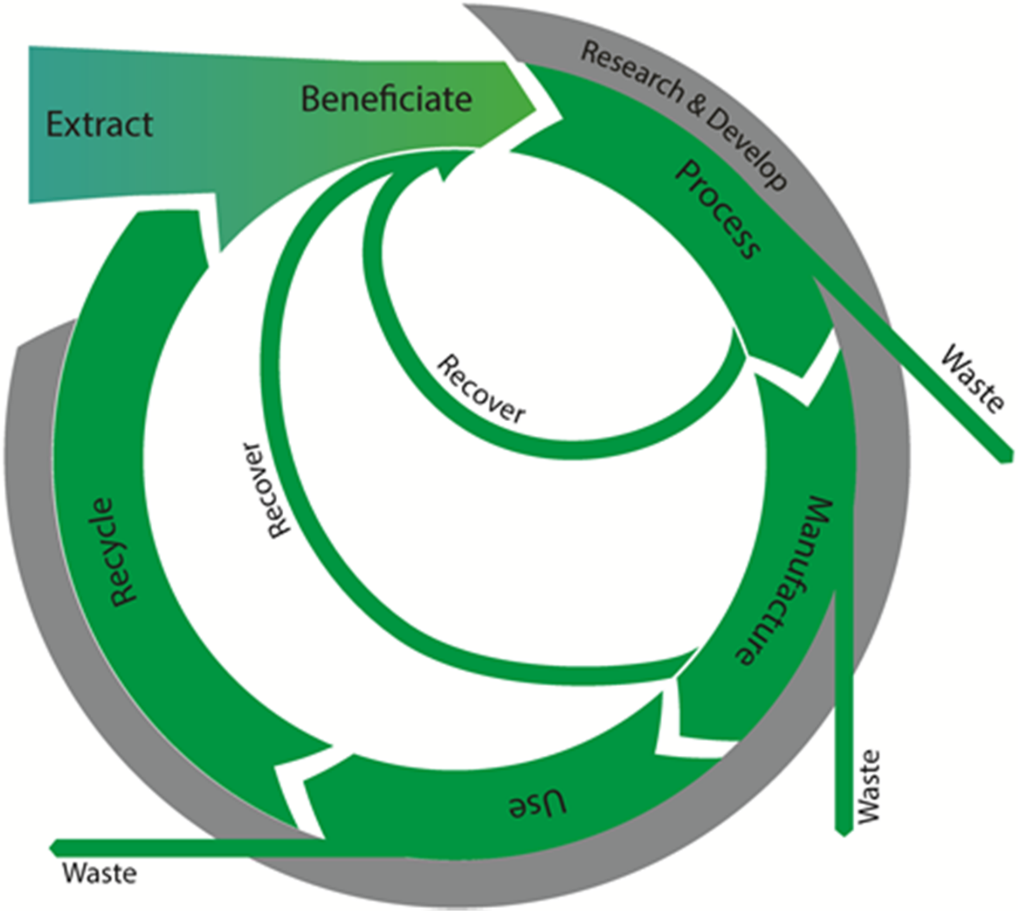
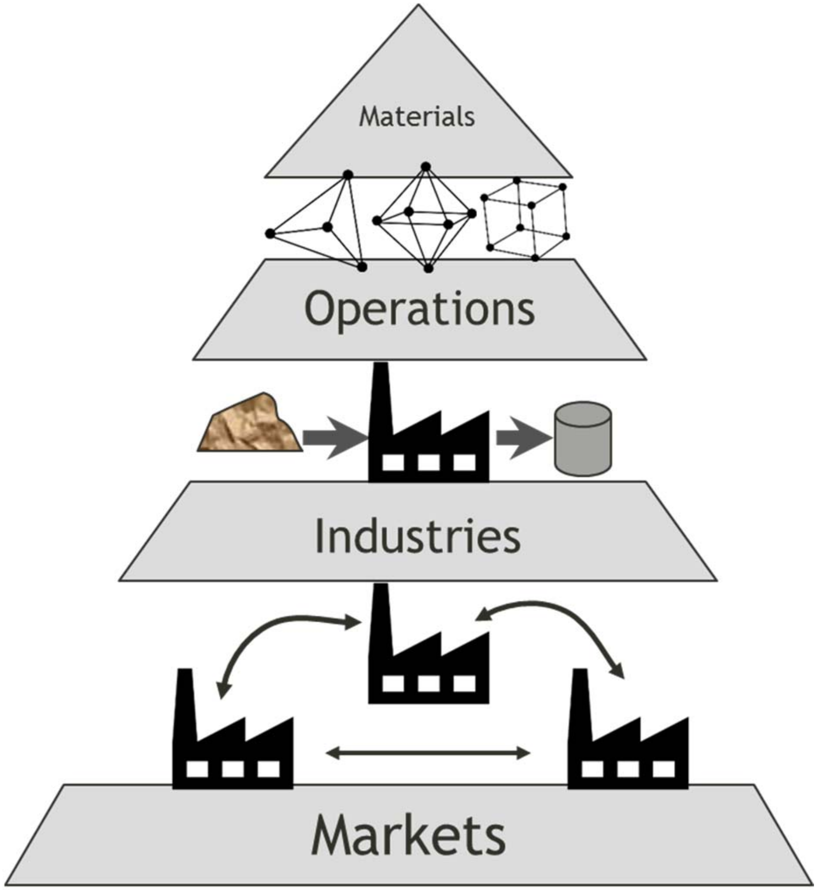
Materials Science &
Engineering

Informing design of resource-effective materials, processes and systems

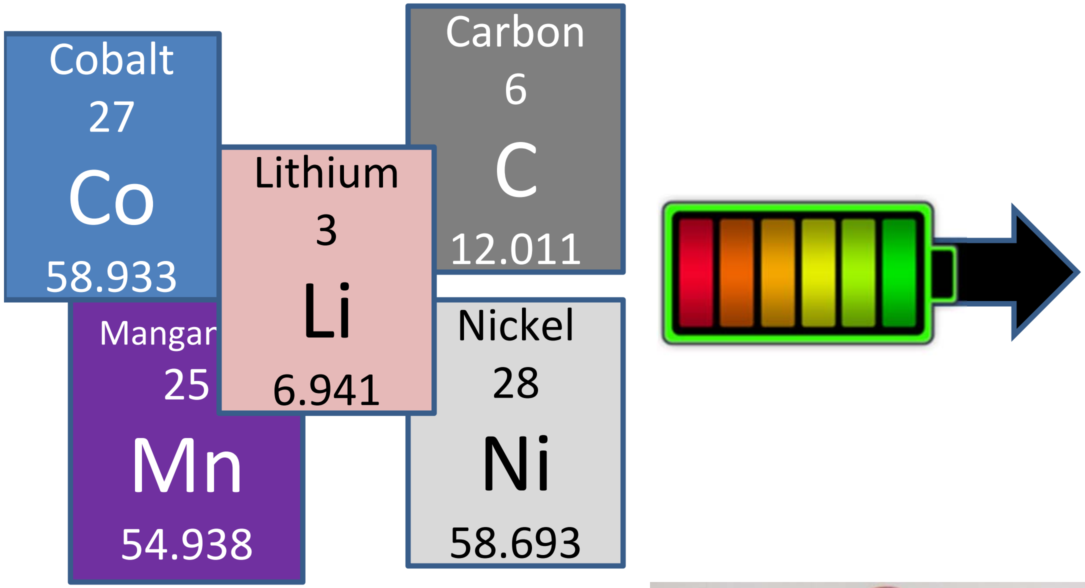
Resource-effective decision making for design of materials, operations, industries, and systems

Materials do not exist in isolation, they are part of complex networks.





Analysis of Potential Supply Chain Bottlenecks in Metals for Li-ion batteries



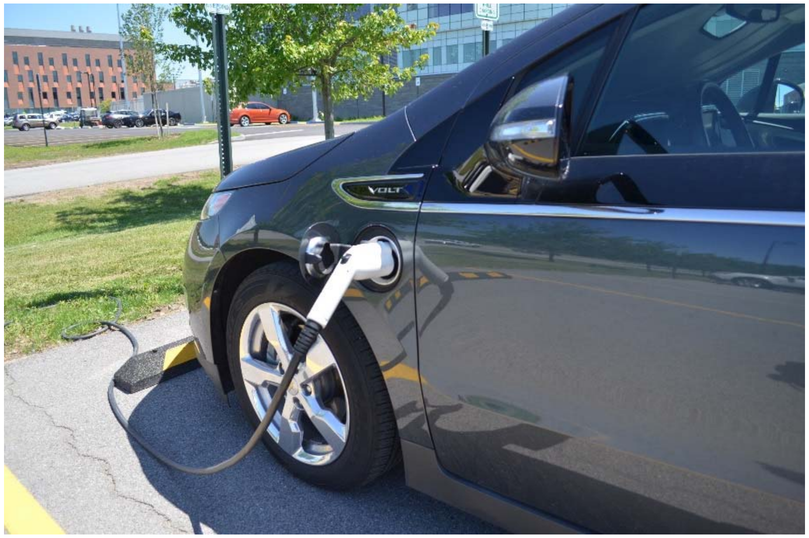
Cobalt
27
Co
58.933

Mangar
25
Mn
54.938

Lithium
3
Li
6.941

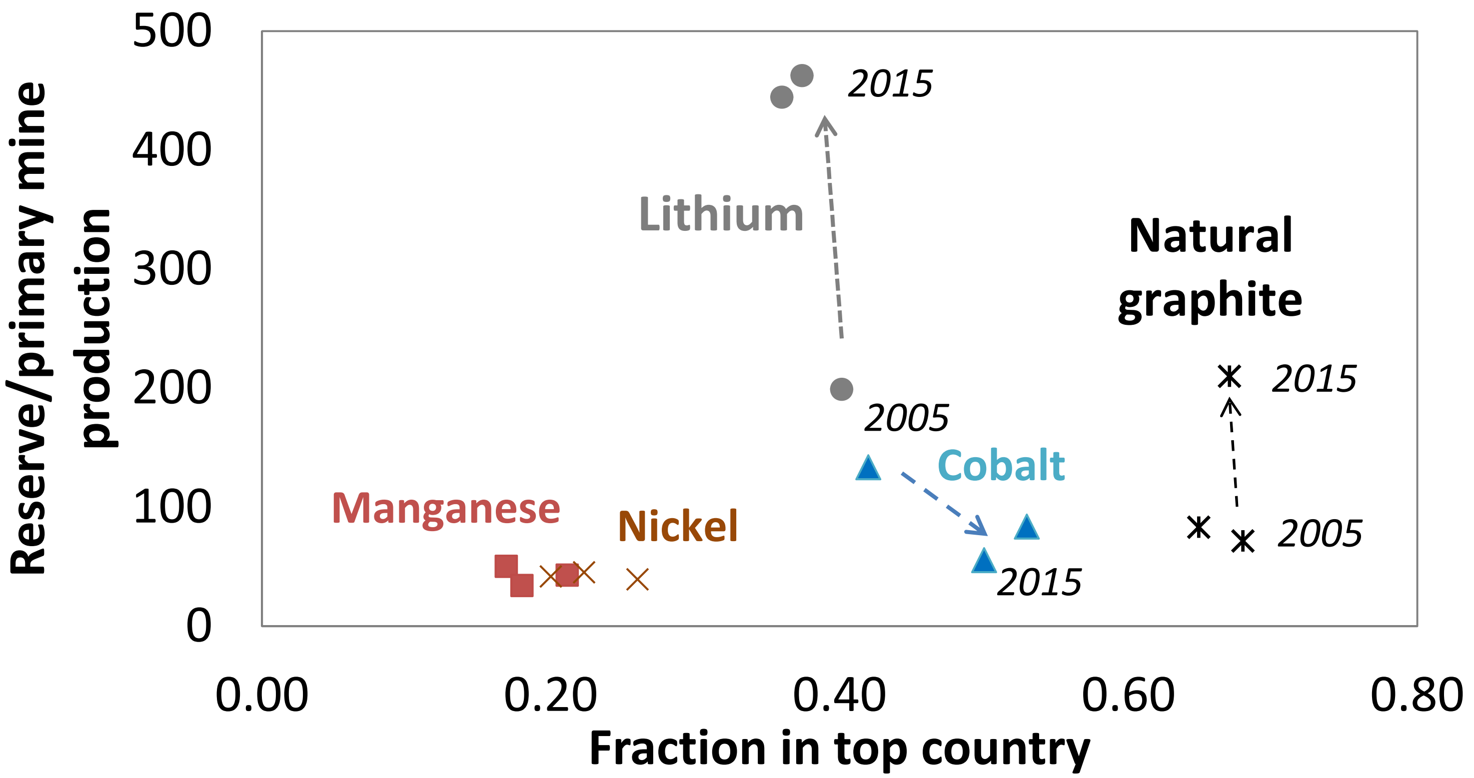
Carbon
6
C
12.011

Nickel
28
Ni
58.693



Joule 2017

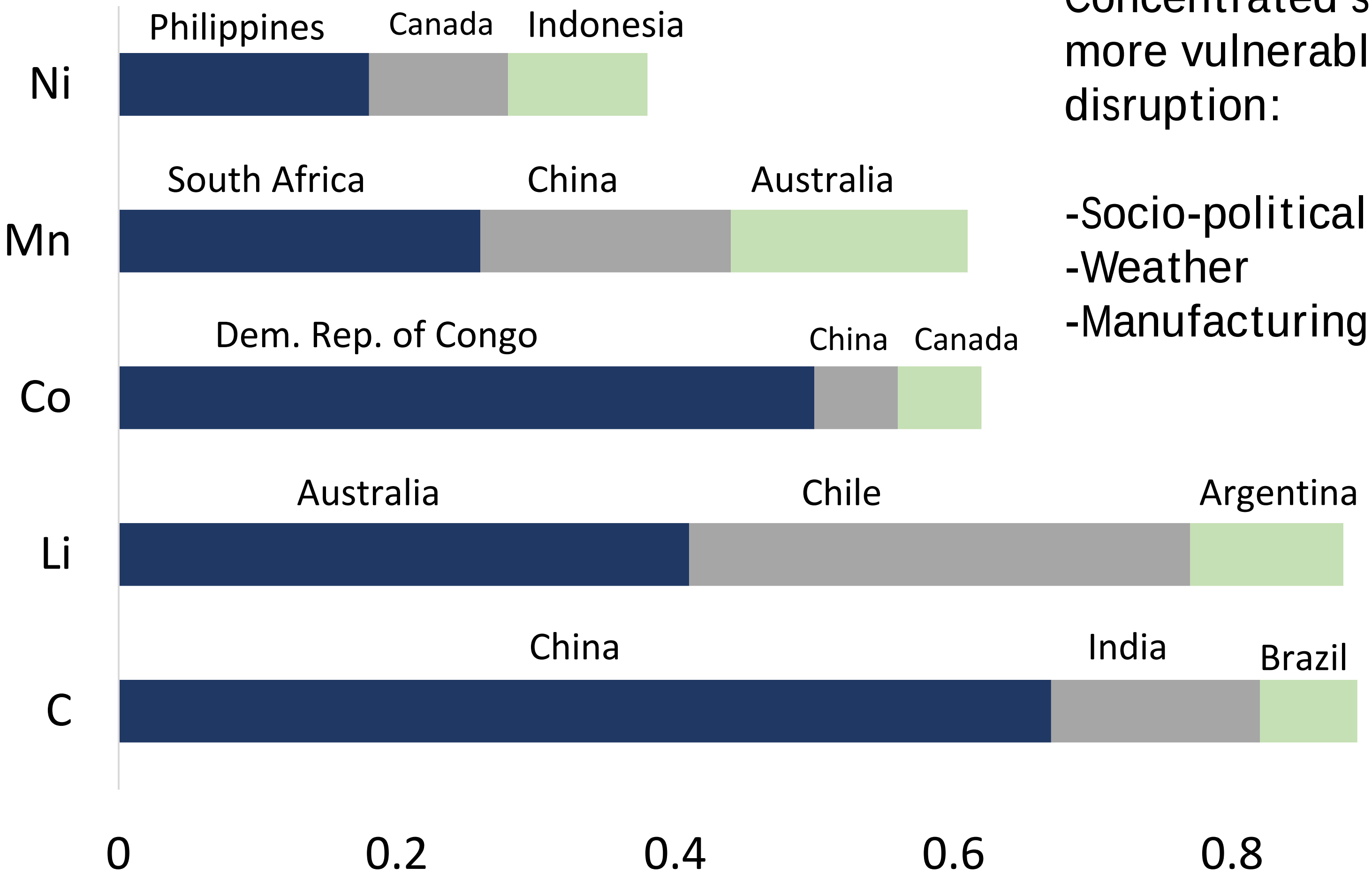
Resource restrictions for relevant materials



Static depletion above 30 years for all

Ni and Mn index is relatively constant indicating that the economics of demand drive the supply towards continued economical extraction.

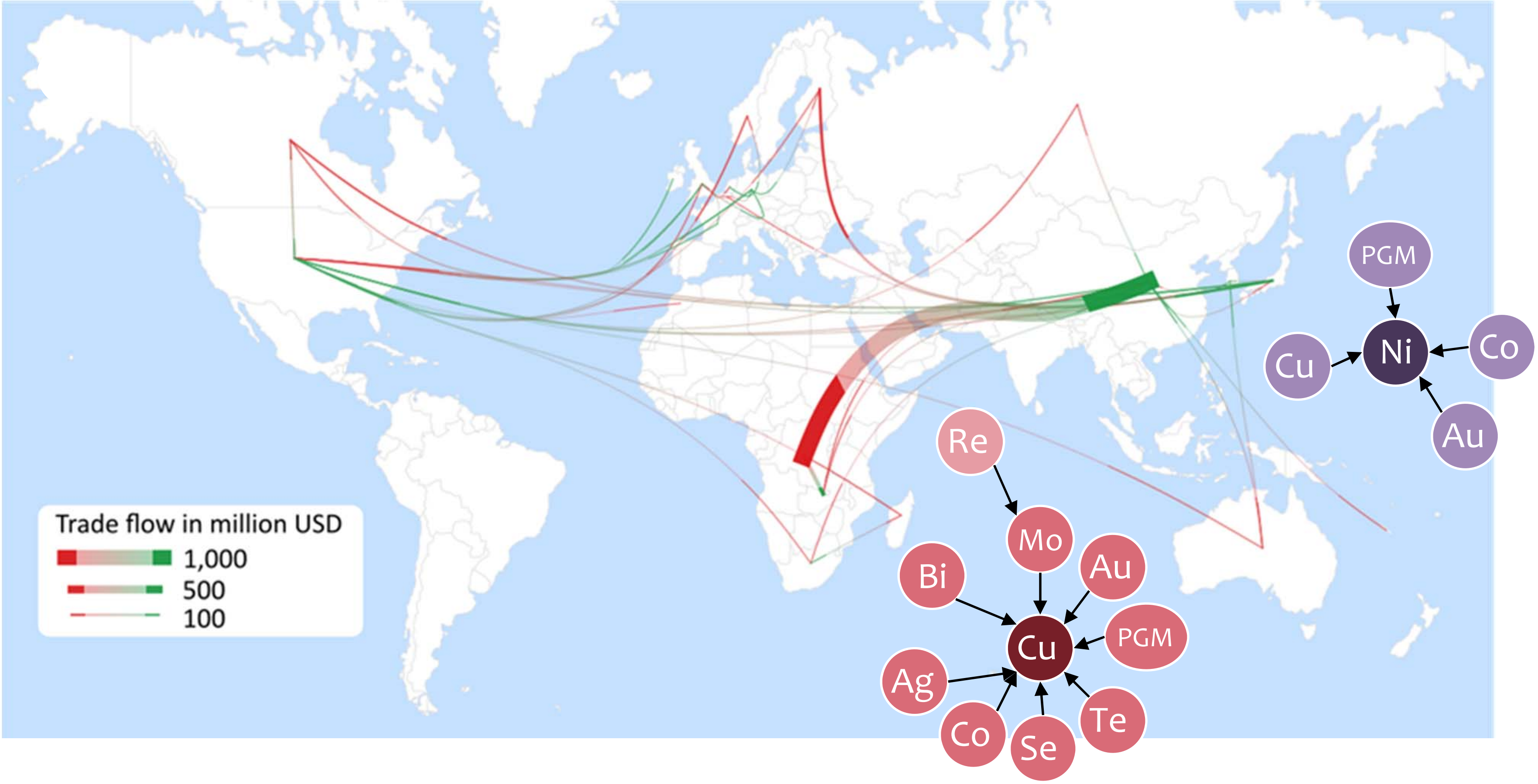
Geographic concentration for relevant materials



Concentrated supply chain more vulnerable to disruption:

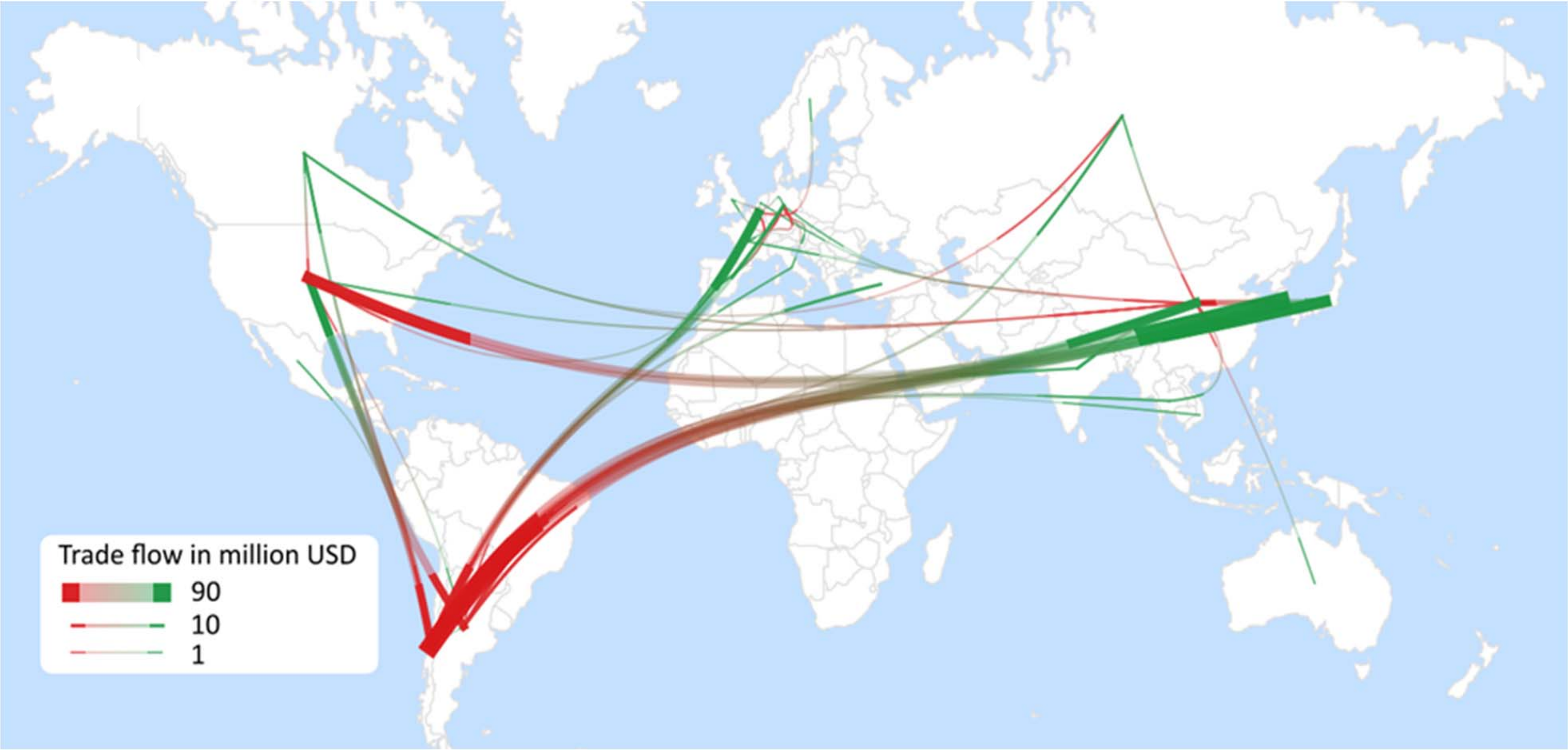
-Socio-political upheaval
-Weather
-Manufacturing bottlenecks

Cobalt supply chain focuses on few dominant players



Co globally concentrated in mining, but it is also geographically concentrated in refining

Lithium supply chain is more diversified



Lithium carbonate recovered via multiple routes and geographically less concentrated

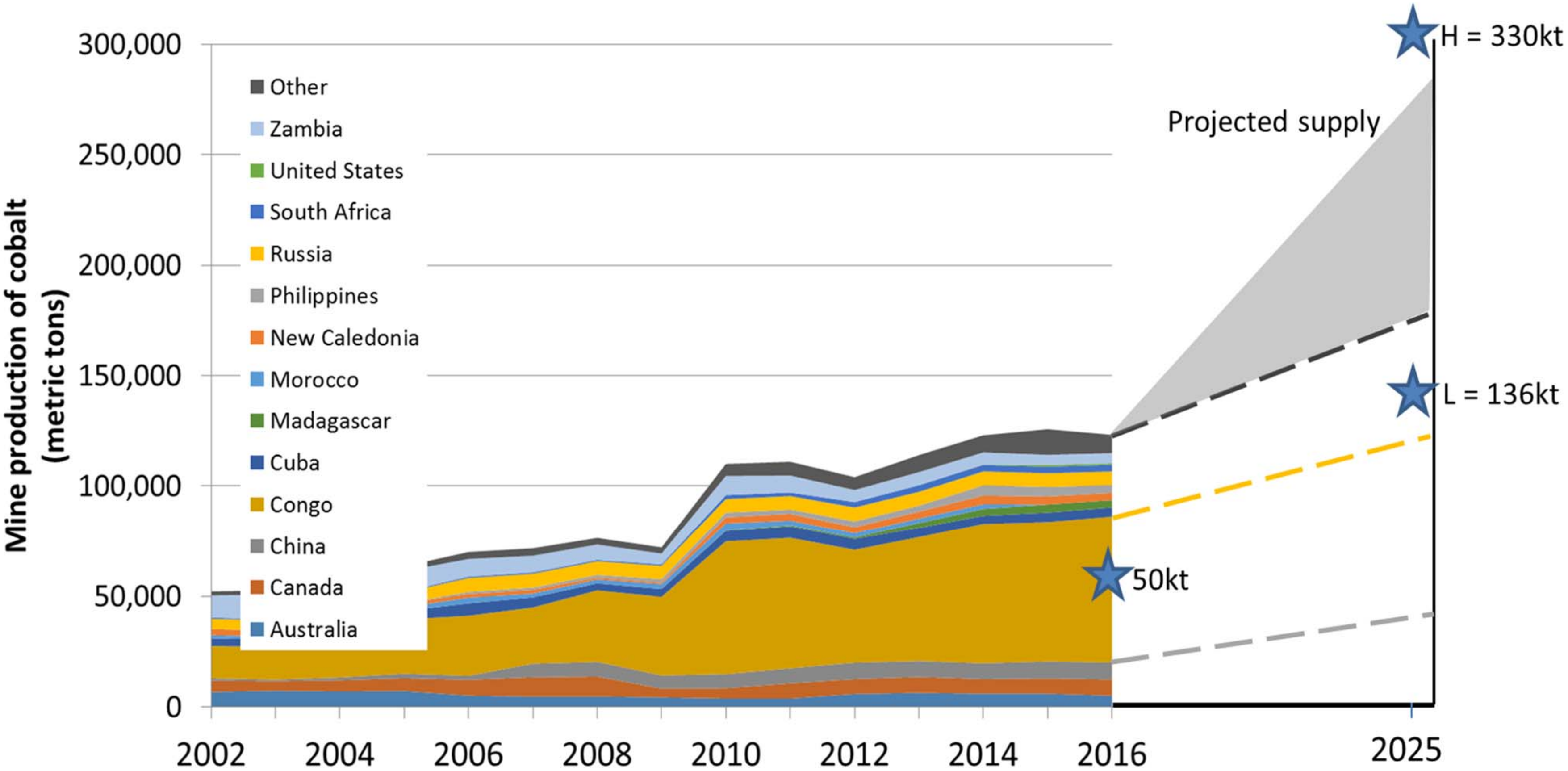
Resource and reserve estimates are still expanding

Amount of material needed per kWh varies by chemistry

	Use	Li	Co	Ni	Mn	Graphitic carbon
Lithium cobalt oxide	electronics	0.113	0.959	0	0	~1.2*
Lithium nickel cobalt aluminum oxide	Auto, grid, other	0.112	0.143	0.759	0	
Lithium nickel manganese cobalt oxide NMC-111		0.139	0.394	0.392	0.367	
NMC-622		0.126	0.214	0.641	0.200	
NMC-811		0.111	0.094	0.750	0.088	

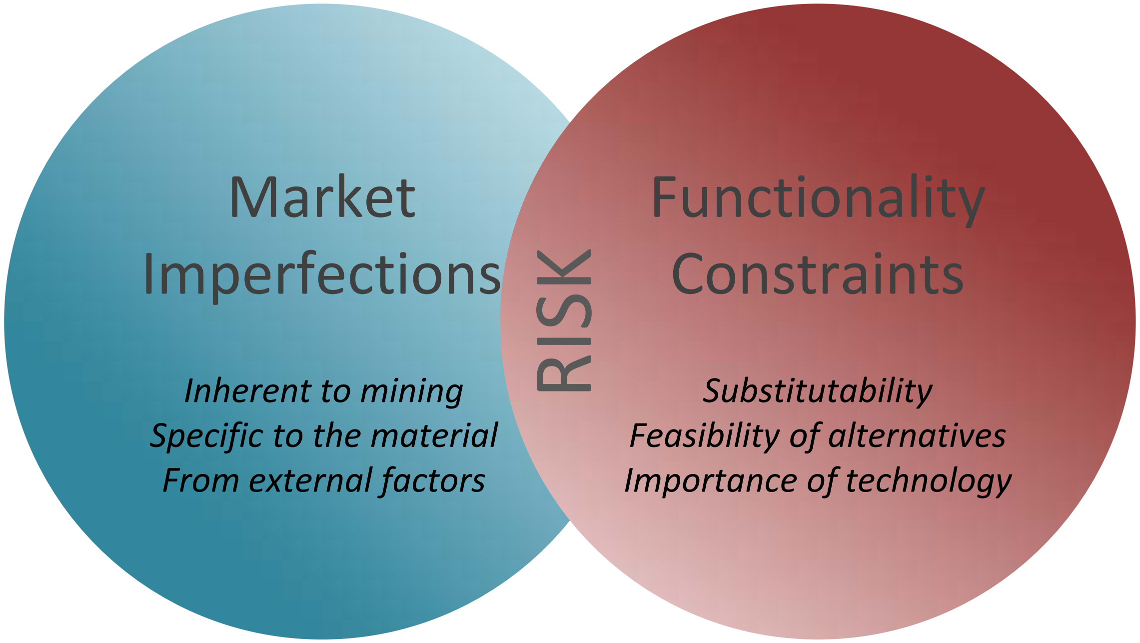
Current metal required in kg/kWh
* literature values

Focus on cobalt demand and supply



What is materials criticality?

Criticality ≠ Scarcity!



Market Imperfections

Inherent to mining
Specific to the material
From external factors

RISK

Functionality Constraints

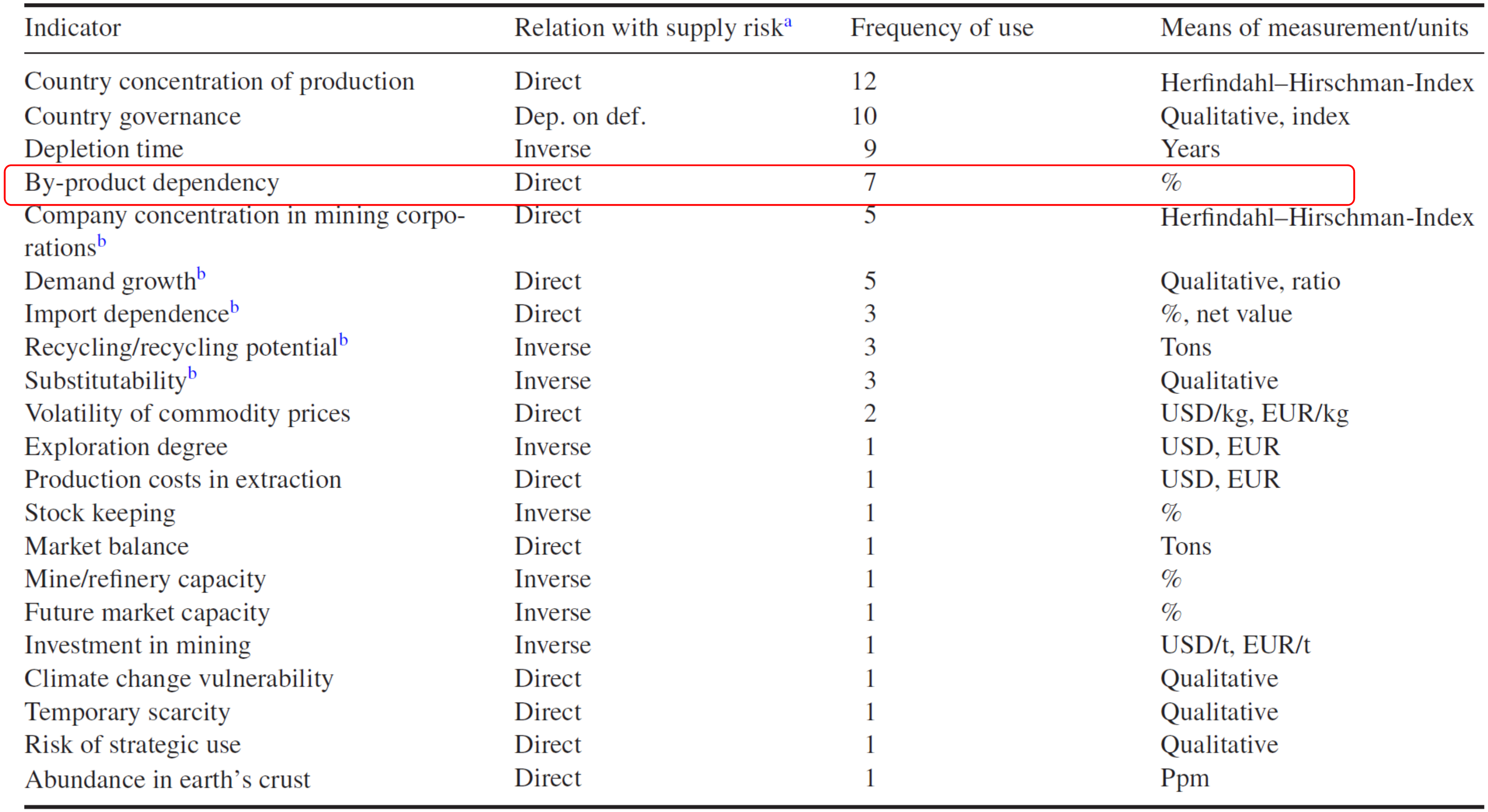
Substitutability
Feasibility of alternatives
Importance of technology

Criticality

Risk deemed too high by a decision-maker

Materials availability:

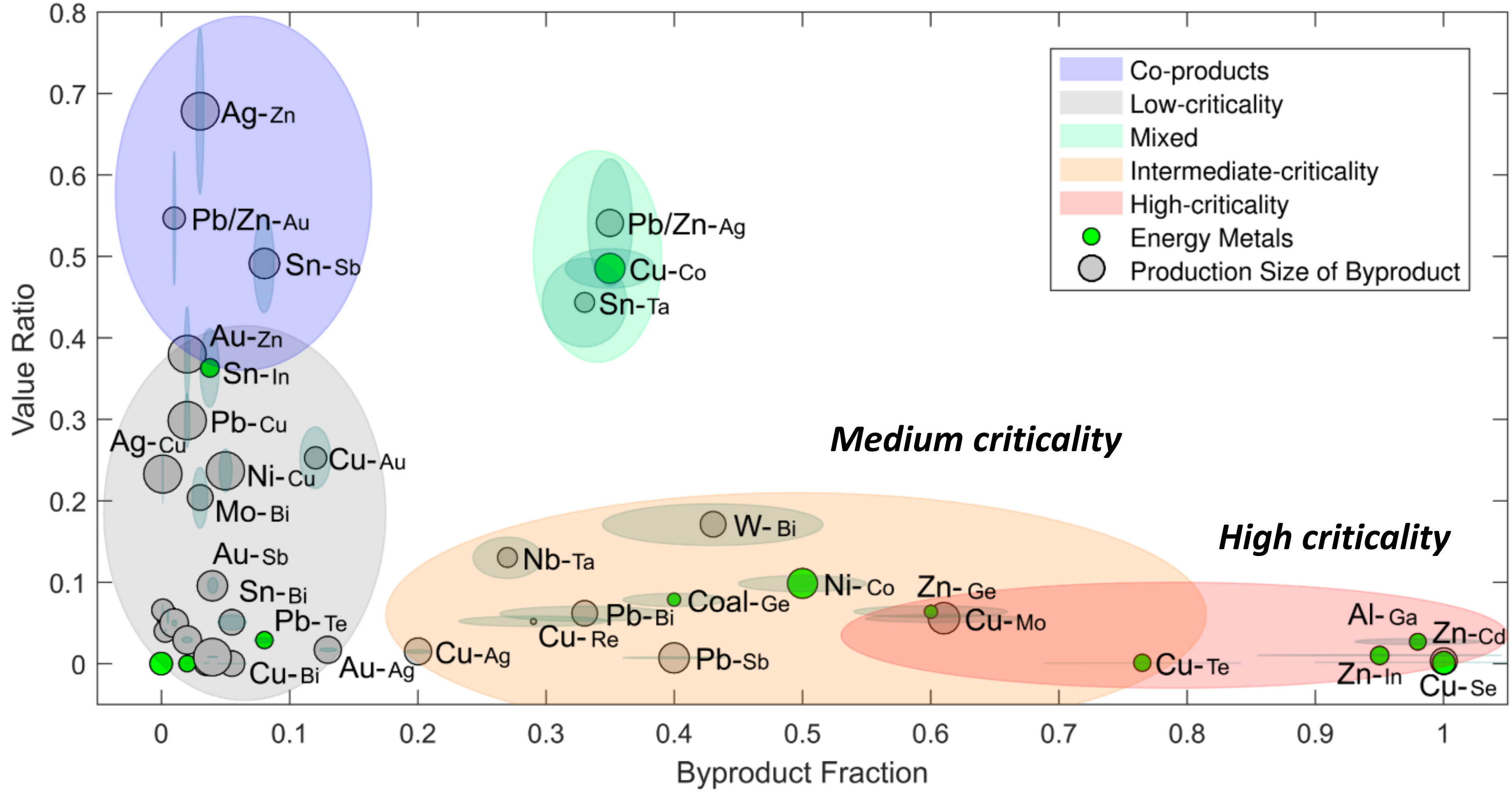
Byproduct dependency used as metric of criticality



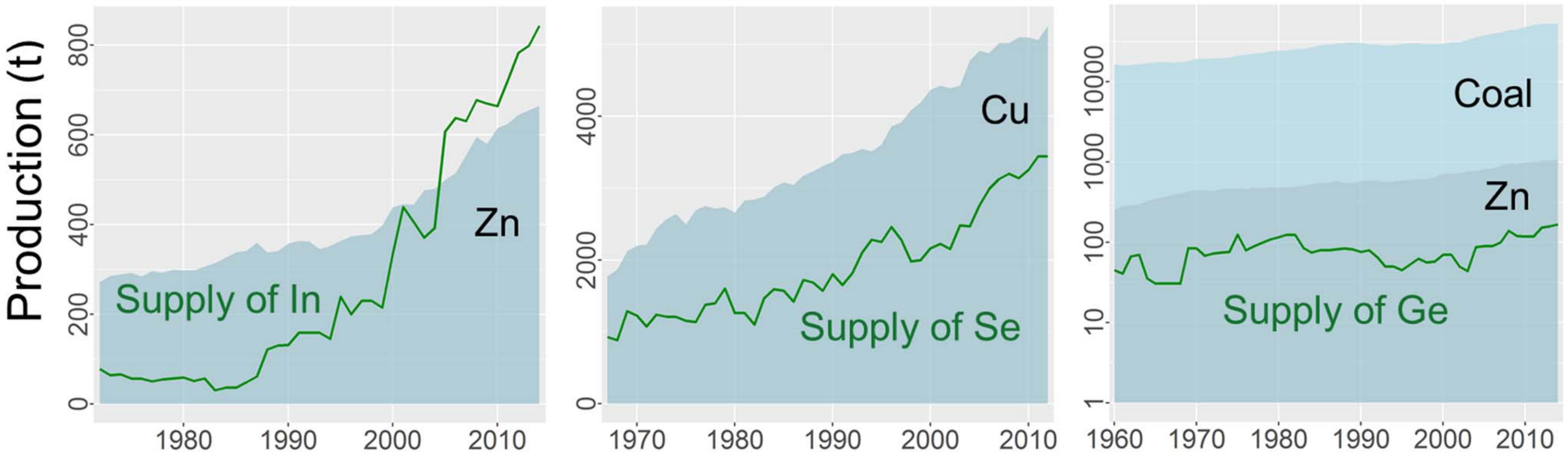
Indicator	Relation with supply risk[a]	Frequency of use	Means of measurement/units
Country concentration of production	Direct	12	Herfindahl–Hirschman-Index
Country governance	Dep. on def.	10	Qualitative, index
Depletion time	Inverse	9	Years
By-product dependency	Direct	7	%
Company concentration in mining corporations[b]	Direct	5	Herfindahl–Hirschman-Index
Demand growth[b]	Direct	5	Qualitative, ratio
Import dependence[b]	Direct	3	%, net value
Recycling/recycling potential[b]	Inverse	3	Tons
Substitutability[b]	Inverse	3	Qualitative
Volatility of commodity prices	Direct	2	USD/kg, EUR/kg
Exploration degree	Inverse	1	USD, EUR
Production costs in extraction	Direct	1	USD, EUR
Stock keeping	Inverse	1	%
Market balance	Direct	1	Tons
Mine/refinery capacity	Inverse	1	%
Future market capacity	Inverse	1	%
Investment in mining	Inverse	1	USD/t, EUR/t
Climate change vulnerability	Direct	1	Qualitative
Temporary scarcity	Direct	1	Qualitative
Risk of strategic use	Direct	1	Qualitative
Abundance in earth's crust	Direct	1	Ppm

(Frenzel et al., 2017)

Criticality classification of byproduct and carrier pairs



Develop and refine metrics to guide decision making



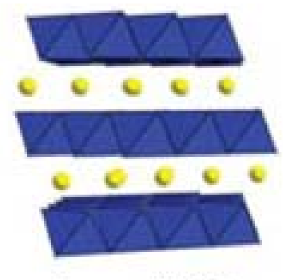
System	Supply elasticity 95% CI	Causes of inelasticity	
Zn-In	(-0.08, 0.29)	Supply limited by production capacity from carrier	Lack of global price setting mechanism
Cu-Se	(-0.03, 0.09)	Supply limit of carrier; Limit of recovery efficiency (~50%)	
Zn/Coal-Ge	(-0.31, 0.36)	National stockpiling strategy	

Byproduct status as indicator of criticality?

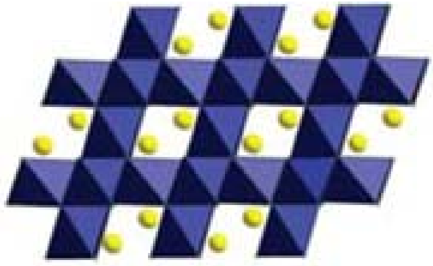
- Sometimes…
- Yes for indium
- Mixed evidence for selenium and germanium's inelastic supply, including:
  - the supply limit of carrier,
  - recovery efficiency limits,
  - lack of a global price-setting mechanism
  - national strategic stockpiling that disrupts market forces.
- Conclusion: Difference between supply and supply potential more indicative of criticality than 'byproduct dependence'

Novel materials development

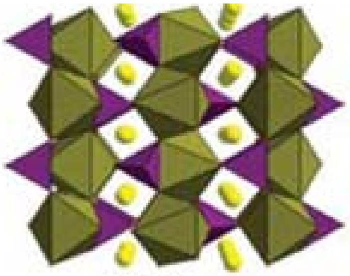
Non-cobalt containing cathodes



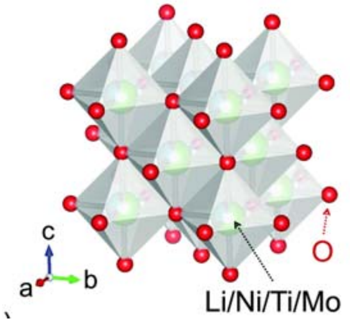
Layered $LiMO_2$
(M=Co, Ni, Mn)

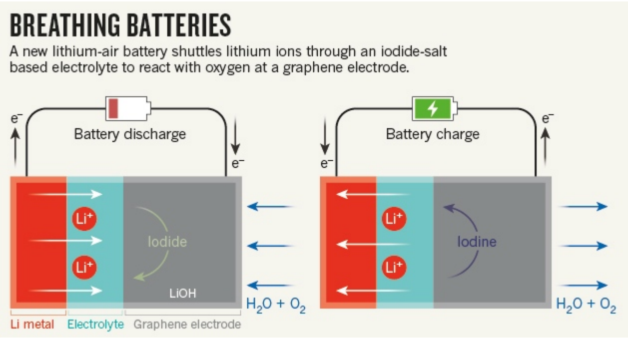


Spinels $LiMn_2O_4$,
$Li_4Ti_5O_{12}$



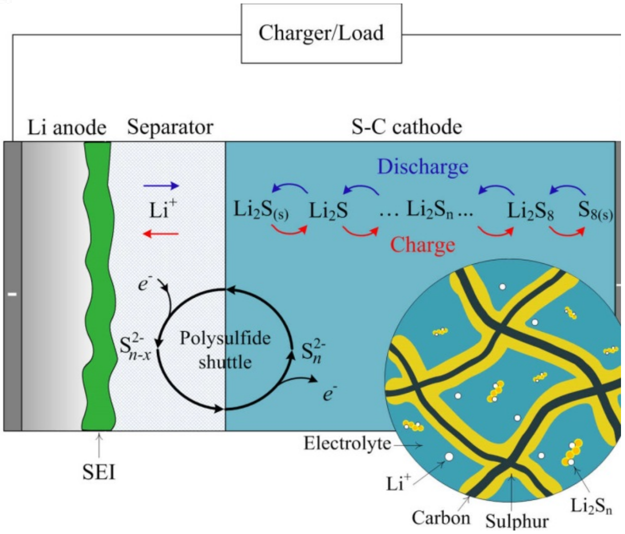
$LiFePO_4$





BREATHING BATTERIES

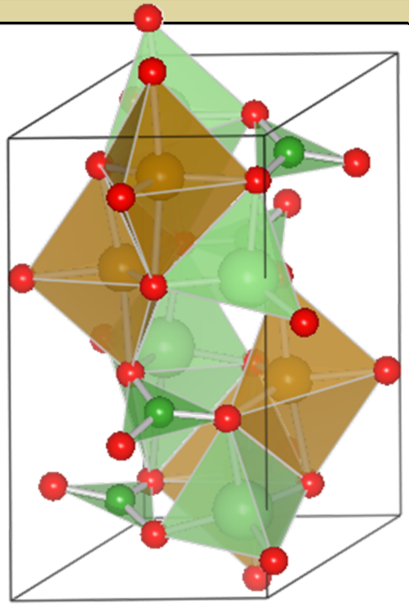
A new lithium-air battery shuttles lithium ions through an iodide-salt based electrolyte to react with oxygen at a graphene electrode.



Li-air, Li-sulfur

Solid state

Computational efforts have accelerated the materials discovery process

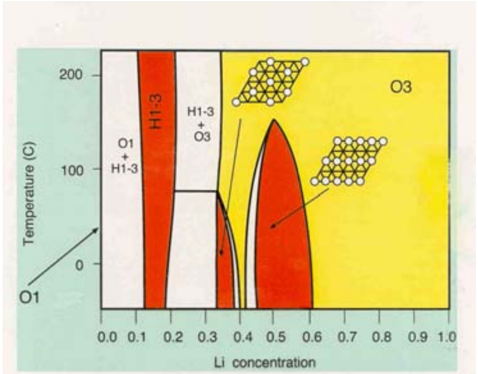


+

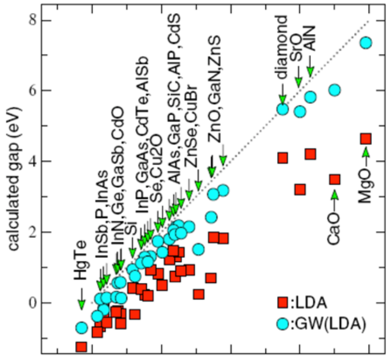
+

$$H=\sum_{i=1}^{N_e}\nabla_i^2+\sum_{i=1}^{N_e}V_{nuclear}(r_i)+\frac{1}{2}\sum_{i}^{N_e}\sum_{j\neq i}^{N_e}\frac{1}{|\boldsymbol{r}_j-\boldsymbol{r}_i|}$$

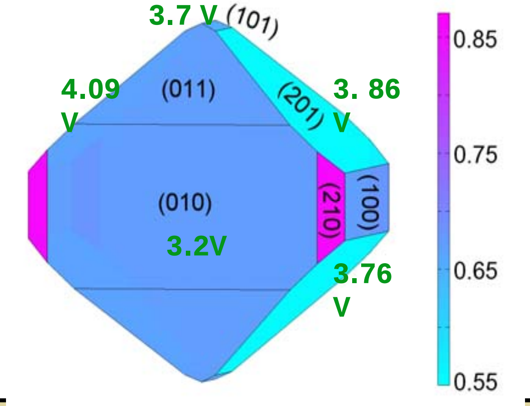
Phase diagrams

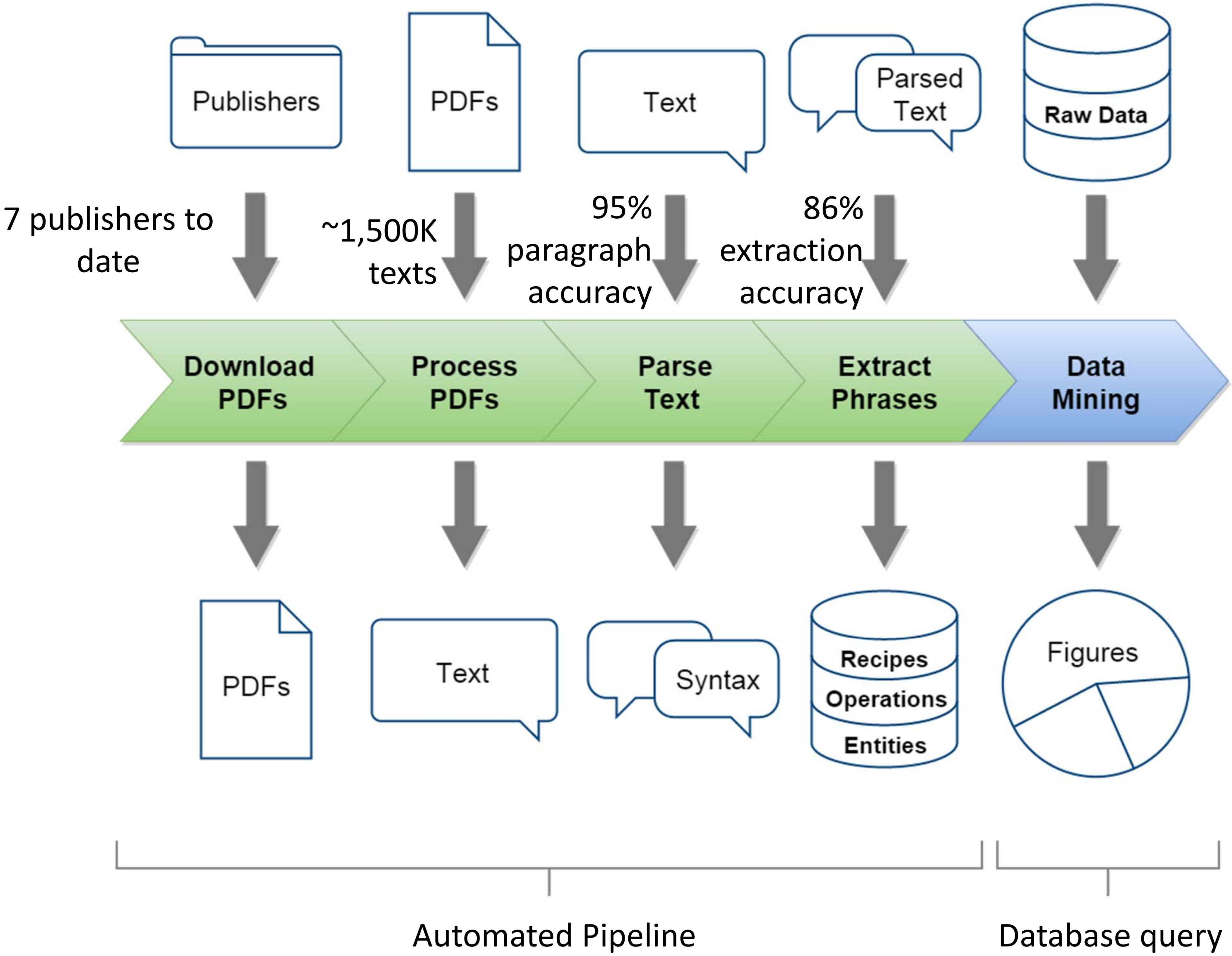


Bandgaps

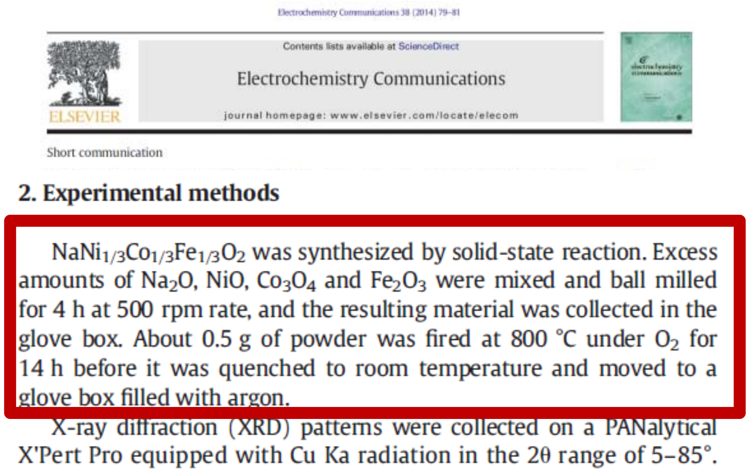


Surfaces




Publishers
PDFs
Text
Parsed Text
Raw Data
7 publishers to date
~1,500K texts
95% paragraph accuracy
86% extraction accuracy
Download PDFs
Process PDFs
Parse Text
Extract Phrases
Data Mining
PDFs
Text
Syntax
Recipes
Operations
Entities
Figures
Automated Pipeline
Database query

Develop recipe database to improve understanding of materials synthesis



Electrochemistry Communications 38 (2014) 79–81

Contents lists available at ScienceDirect

Electrochemistry Communications

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

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Short communication

2. Experimental methods

$NaNi_{1/3}Co_{1/3}Fe_{1/3}O_2$ was synthesized by solid-state reaction. Excess amounts of Na_2O, NiO, Co_3O_4 and Fe_2O_3 were mixed and ball milled for 4 h at 500 rpm rate, and the resulting material was collected in the glove box. About 0.5 g of powder was fired at 800 °C under O_2 for 14 h before it was quenched to room temperature and moved to a glove box filled with argon.

X-ray diffraction (XRD) patterns were collected on a PANalytical X'Pert Pro equipped with Cu Ka radiation in the 2θ range of 5–85°.

Identify hundreds of thousands of manuscripts by target material

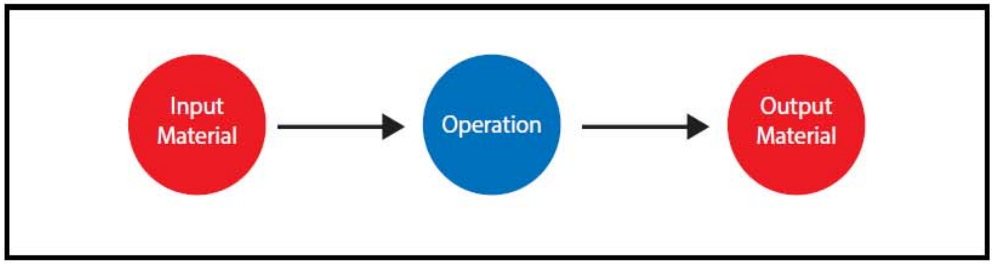
Extract synthesis **text** through machine learning and rule-based methods

$NaNi_{1/3}Co_{1/3}Fe_{1/3}O_2$ was synthesized by solid-state reaction. **Excess amounts** of **Na_2O**, **NiO**, **Co_3O_4** and **Fe_2O_3** were **mixed** and **ball milled** for **4 h** at **500 rpm** rate, and the resulting material was collected in the glove box. About **0.5 g** of powder was fired at **800 °C** under **O_2** for **14 h** before it was **quenched** to **room temperature** and moved to a glove box filled with **argon**.

Generate codified, machine readable database of **recipes**

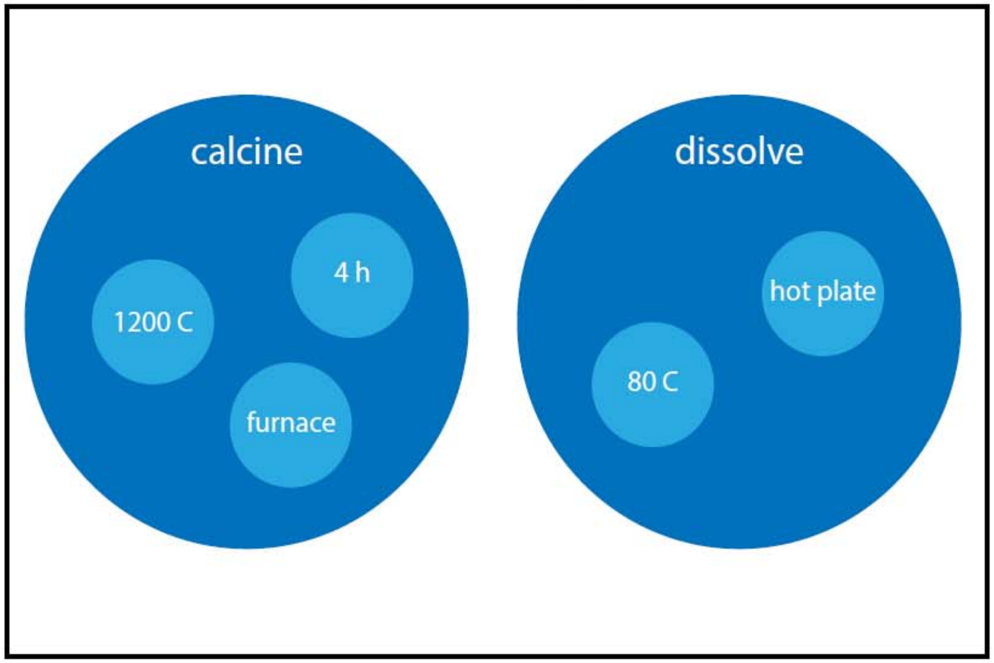
Recipe database

Extracted Synthesis Recipe Schema



Input Material → Operation → Output Material

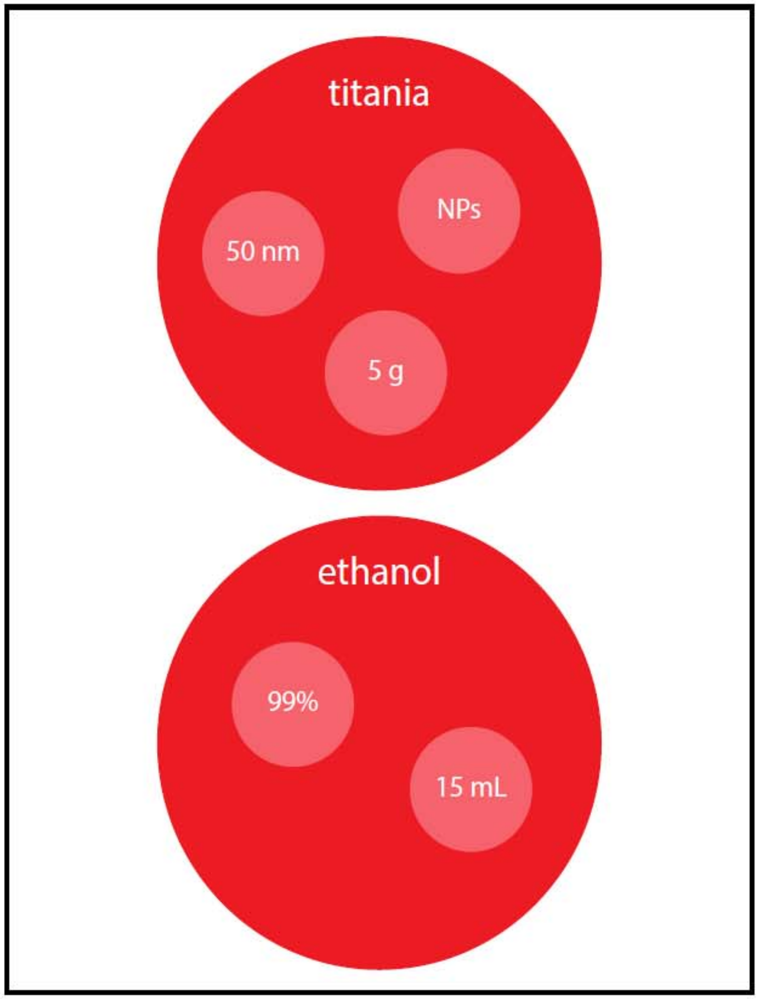
Example Extracted Operations



calcine
1200 C
4 h
furnace

dissolve
80 C
hot plate

Example Extracted Materials

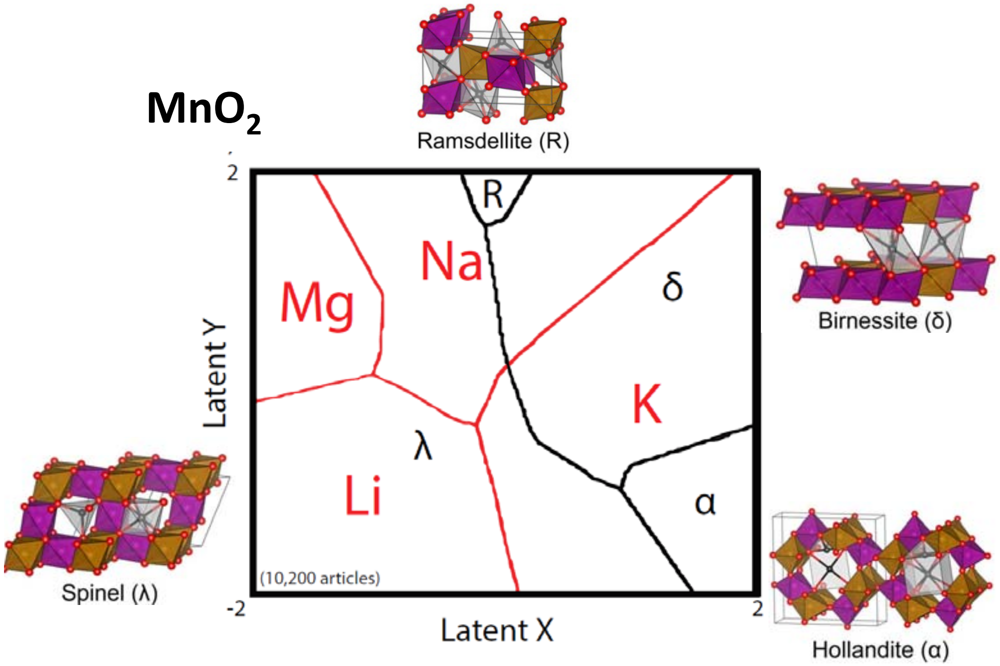


titania
50 nm
NPs
5 g

ethanol
99%
15 mL

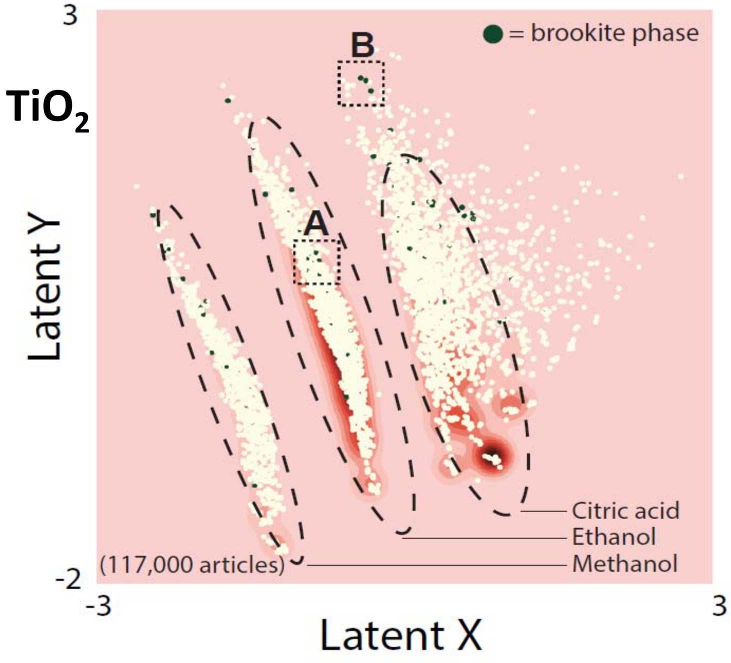
Resource-effective material development: suggesting multiple routes for synthesis

Suggesting synthesis conditions for materials, extend to novel materials



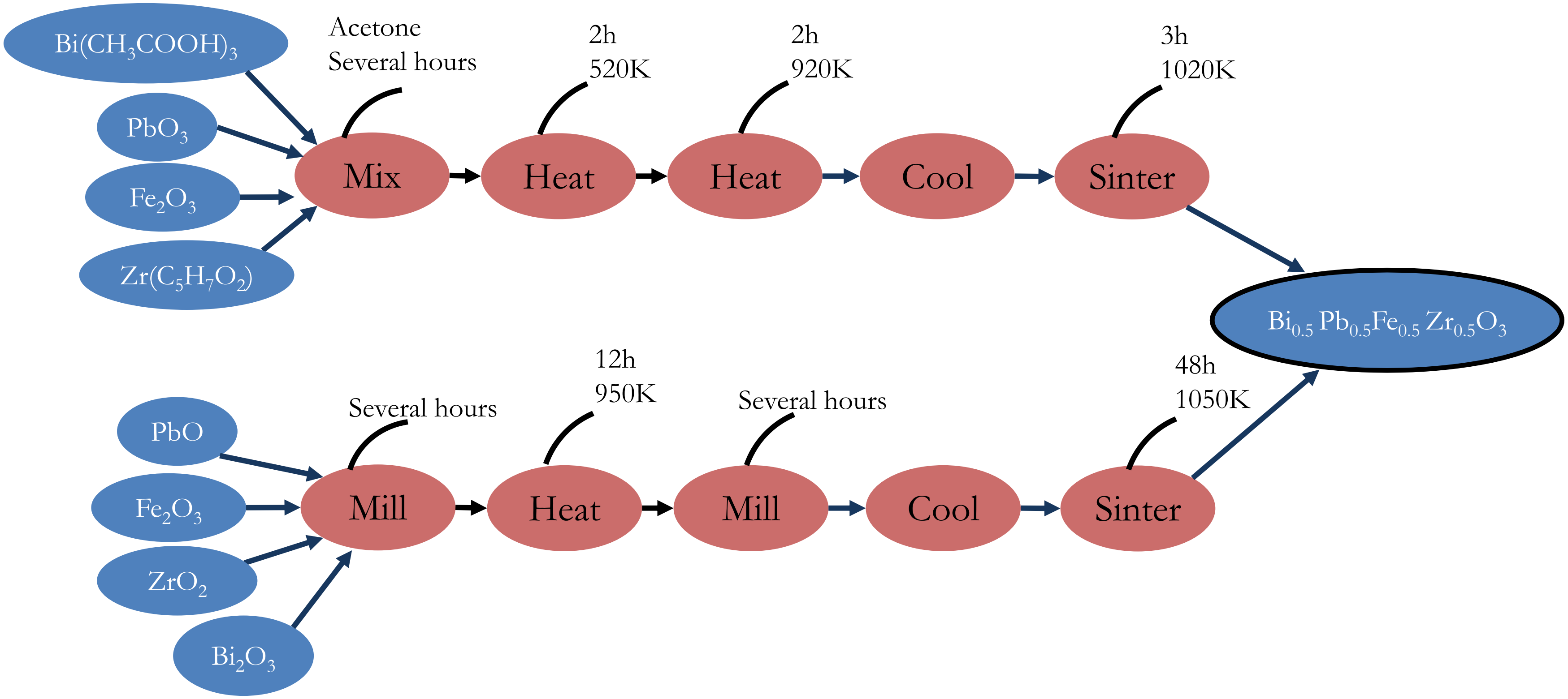
Polymorphs for MnO_2 overlaid with most probable alkali-ion use in synthesis (intercalation-based phase stability)

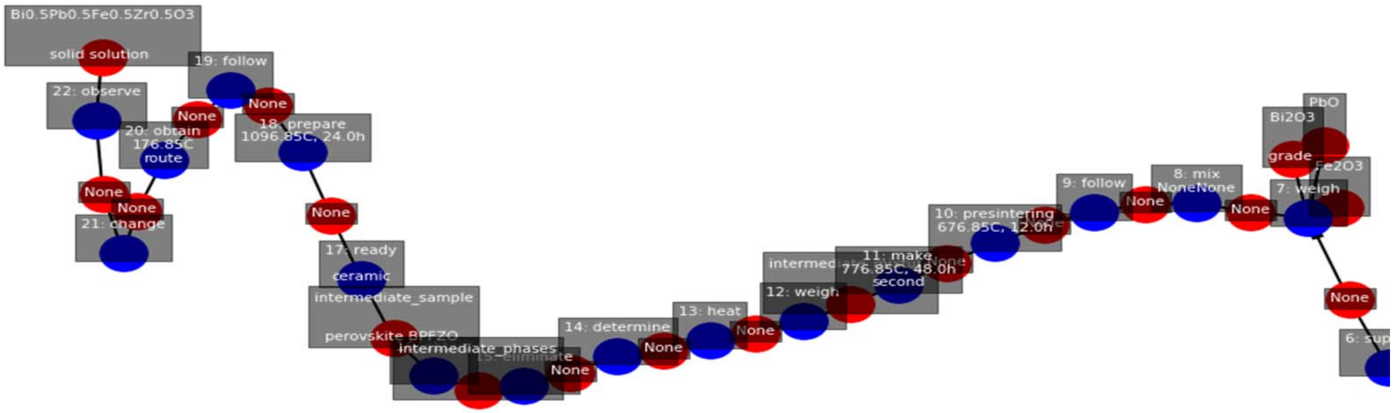
Clustering of latent space points to role for NaOH and ethanol in brookite synthesis

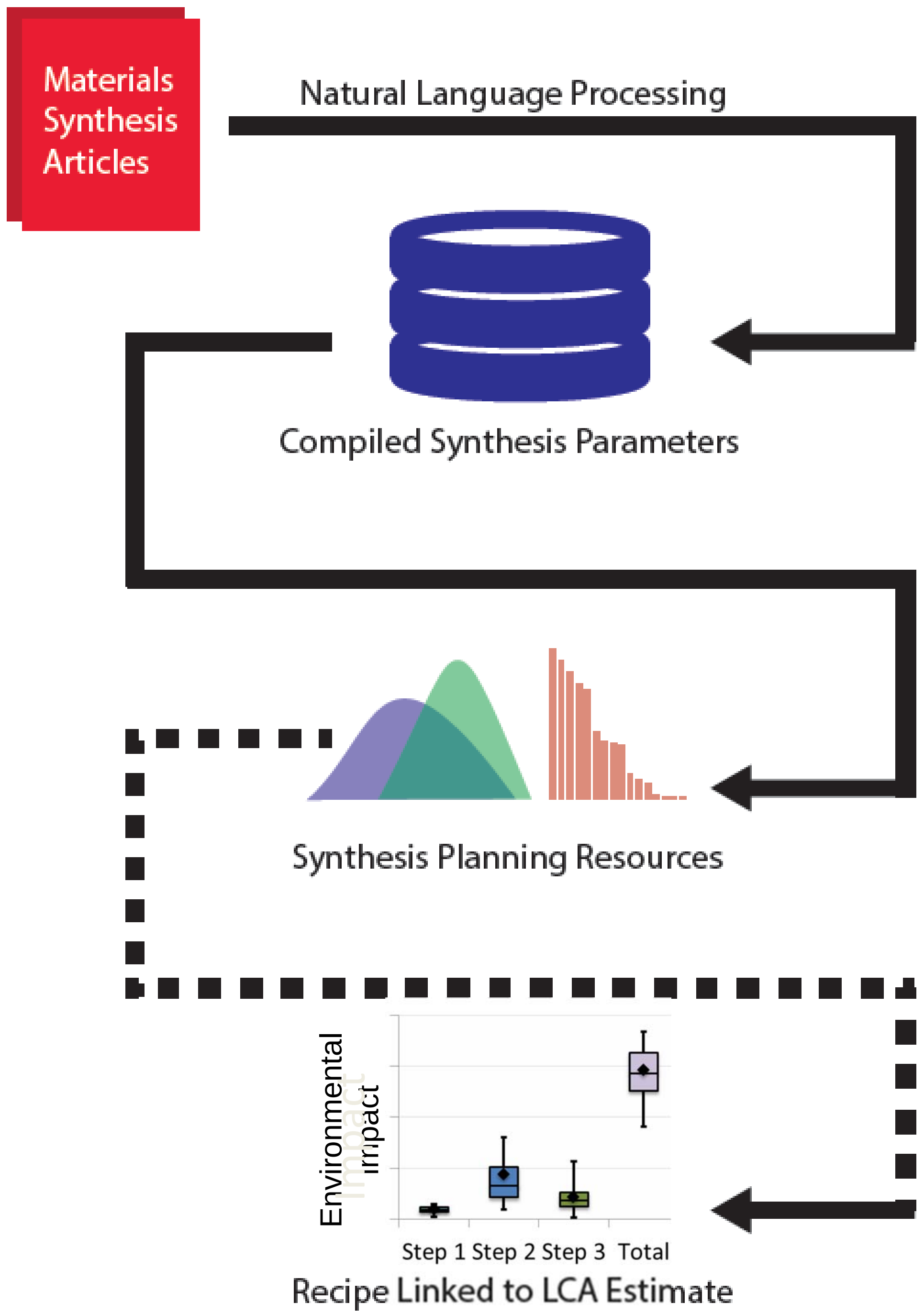


Scientific Data, 2017
Chem. Of Materials, 2017
npj Computational materials, accepted

Generate recipes






Materials Synthesis Articles
Natural Language Processing
Compiled Synthesis Parameters
Synthesis Planning Resources
Environmental impact
Step 1
Step 2
Step 3
Total
Recipe Linked to LCA Estimate

Resource-effective performance of materials

- Systems thinking divorced from materials science and vice versa masks opportunities
  - As system, material, and process complexity increases need novel ways to analyze problems
- Materials have critical role in solving key economic and environmental problems
  - Solutions that account for scale are needed to address the impact of materials use

Thank you

olivetti.mit.edu

Collaborators:
Prof. Gerbrand Ceder,
Prof. Andrew Mccallum
Prof. Stefanie Jegelka
Michael Laracy,
Dr. Thomas Poinot,
Prof. John Ochsendorf,
Prof. Hamlin Jennings

Thank you

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