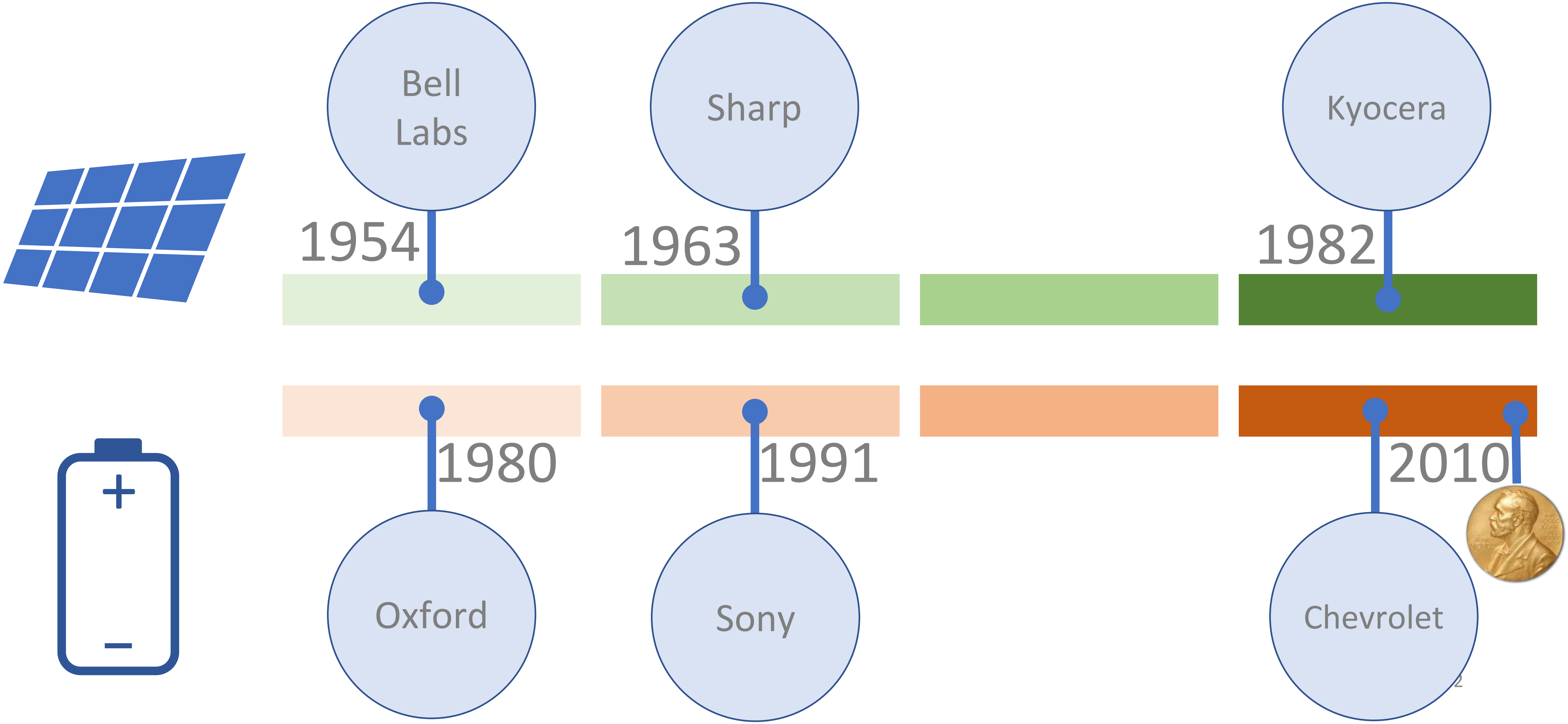
A brief glimpse at a role for data science in GHG mitigation pathways, materials focus

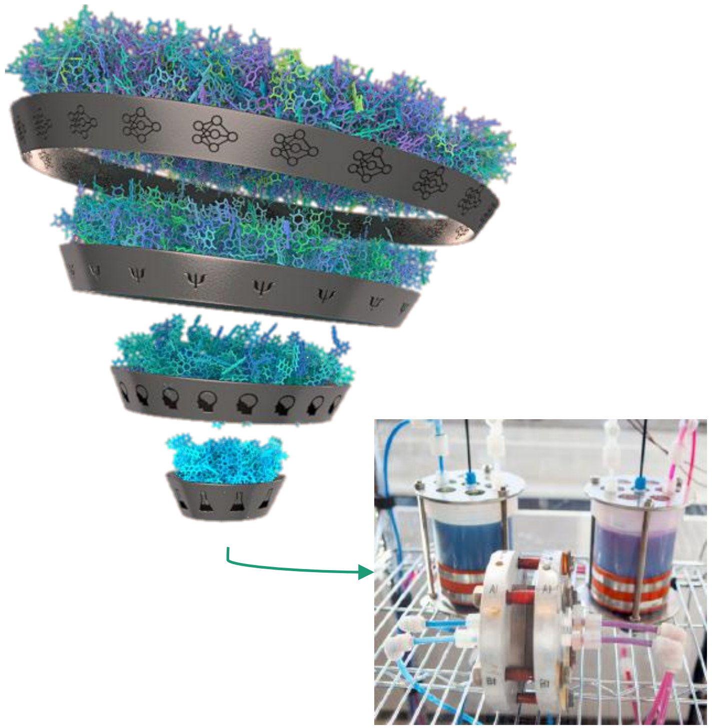
Elsa Olivetti

Department of Materials Science & Engineering

Scale up time measured in decades



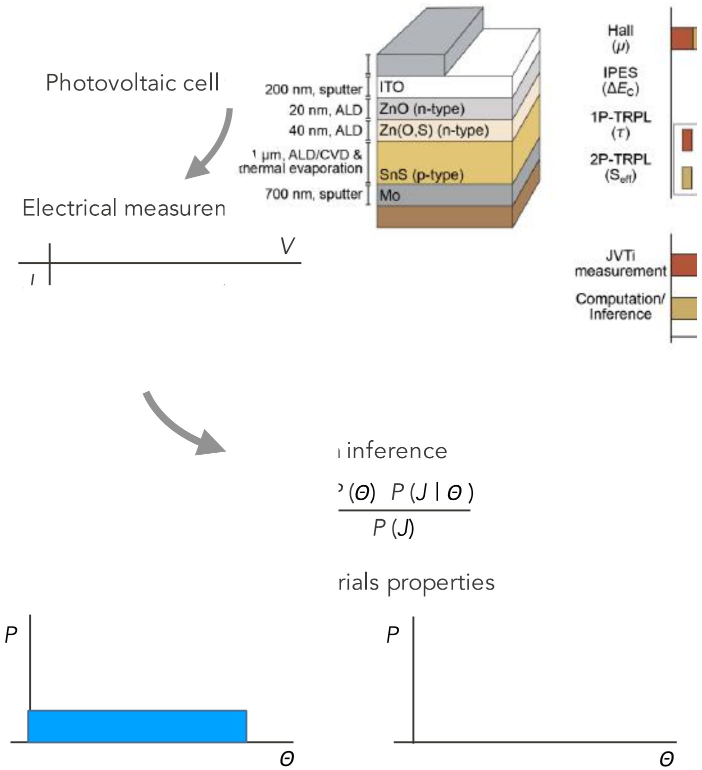
Vision for computer aided, data-driven materials development



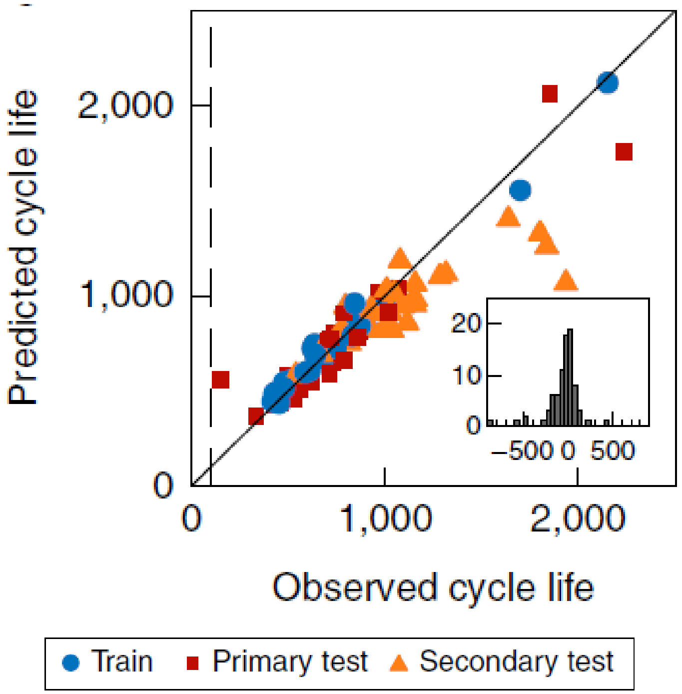
High-throughput virtual screening for promising materials

G-B. et al. *Nature Materials* 2016

Device optimization and high-throughput experimentation

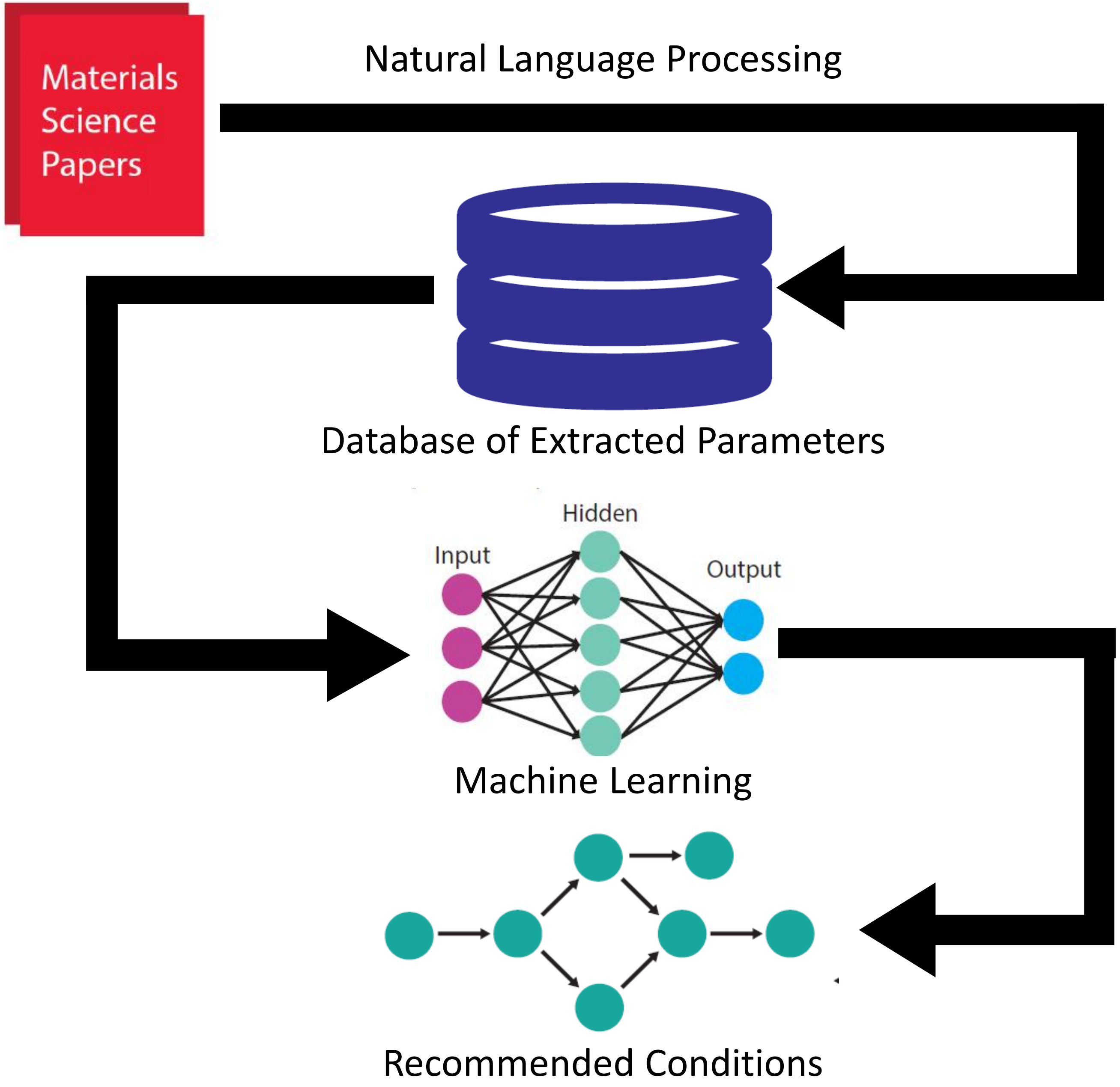


R.E. Brandt et al. *Joule* 2017



Predicting lifetime of complex, nonlinear systems such as lithium-ion batteries

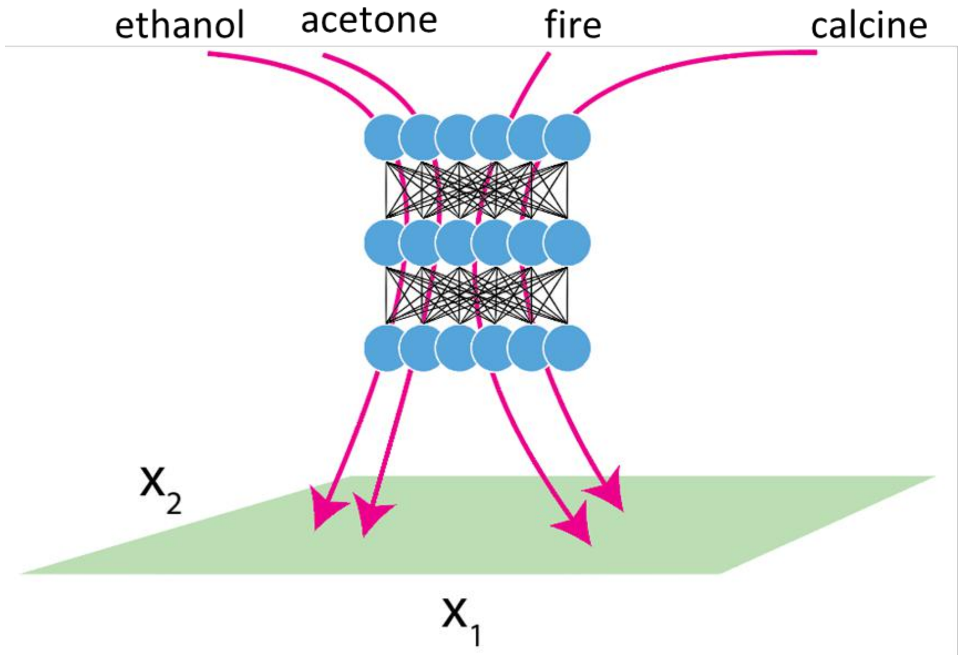
Severson et al. *Nature Energy* 2019


Materials Science Papers
Natural Language Processing
Database of Extracted Parameters
Hidden
Input
Output
Machine Learning
Recommended Conditions

This is a semi-supervised problem

Unsupervised word embeddings

Projections of words into real-value vectors where synonyms are projected to nearby coordinates



Supervised classification

Electrochemistry Communications 38 (2014) 79–81

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ELSEVIER

Short communication

Electrochemical properties of $NaNi_{1/3}Co_{1/3}Fe_{1/3}O_2$ as a cathode material for Na-ion batteries

CrossMark

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1. Introduction

Na-intercalation batteries are appearing as an important alternative to Li intercalation systems, and rapid progress has been made on developing high capacity cathode materials [1]. It has become clear that the Na analogues of the successful layered $LiMO_2$ electrodes behave very differently from their Li equivalents [2]. The large difference in ionic radius between Li and Na provides a stronger tendency for the Na compounds to form in the layered structure [3–7], and layered Na_xMO_2 (M = Ti, V, Cr, Mn, Fe, Co, Ni) [4,8–17], as well as several Na compounds with mixed transition metals, $Na_xNi_{0.6}Co_{0.4}O_2$, $Na_xNi_yMn_{1-y}O_2$, $Na_xTi_yMn_{1-y}O_2$, $Na_xFe_{0.5}Mn_{0.5}O_2$, $NaFe_{0.5}Co_{0.5}O_2$, $NaNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ and $NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$ [18–27], all show electrochemical activity.

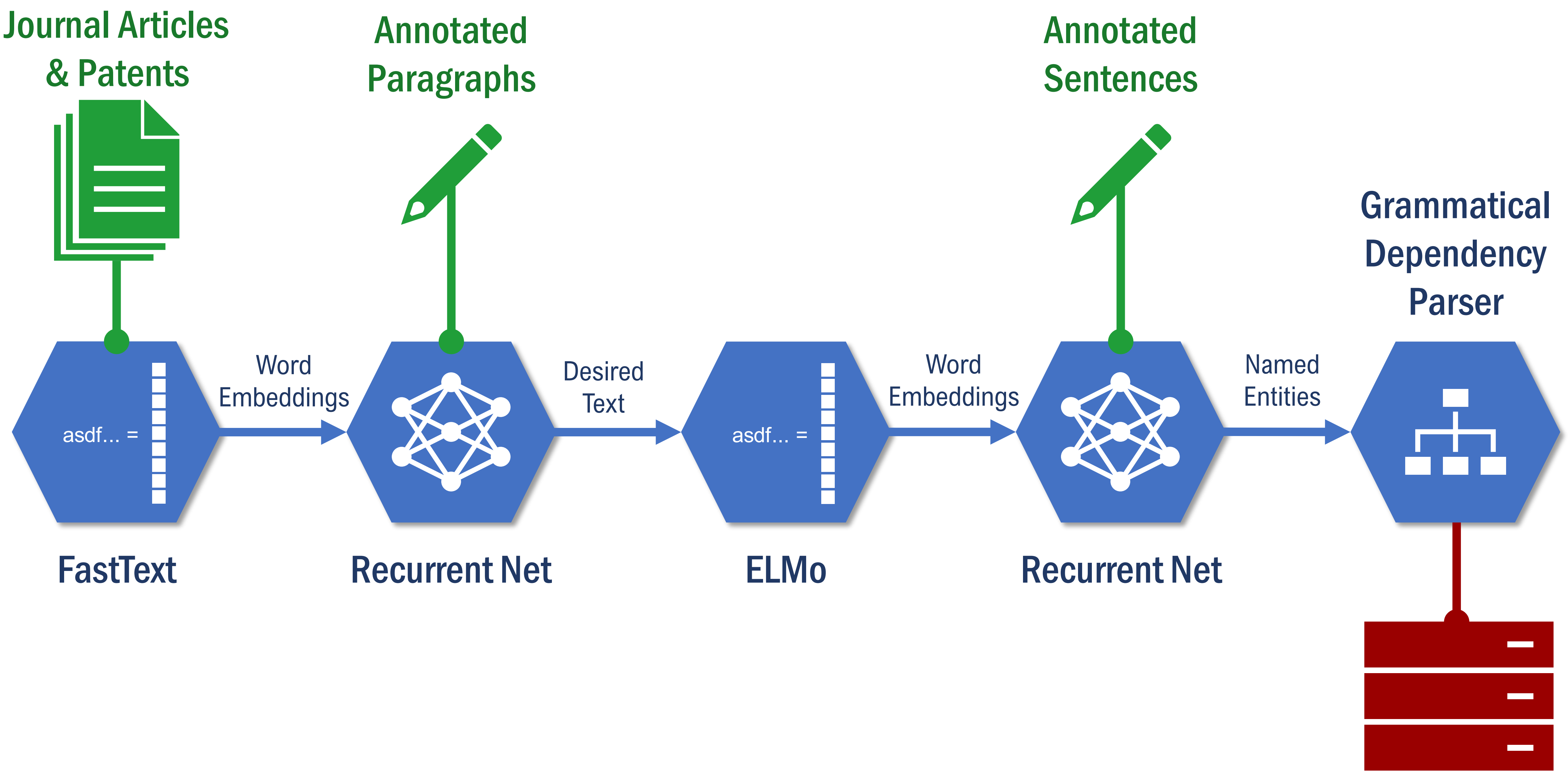
In this paper, we report the synthesis and electrochemical performance of $NaNi_{1/3}Fe_{1/3}Co_{1/3}O_2$ as a novel Na intercalation cathode material. The only layered materials in which three transition metals are mixed in the literature are $NaNi_{1/3}Fe_{1/3}Mn_{1/3}O_2$ [26] and $NaNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ [24], and their capacity is limited to about

material is de-sodiated the Fe and Co are first oxidized to 4+ while the Ni goes through two oxidation steps to reach a final oxidation state in the fully de-sodiated structure of Co^{4+}, Fe^{4+} and Ni^{4+}.

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.

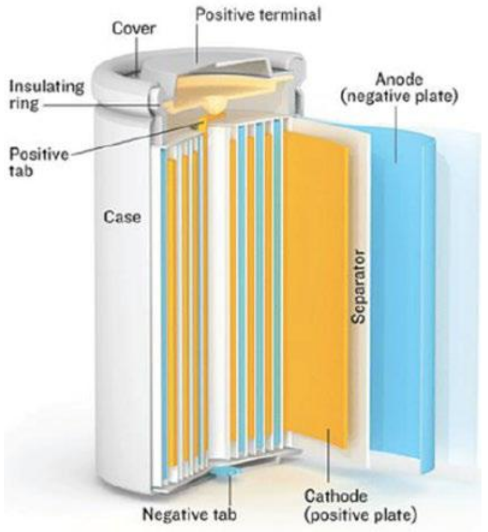
X-ray diffraction (XRD) patterns were collected on a PANalytical X'Pert Pro equipped with Cu Ka radiation in the 2θ range of 5–85°. All the samples were sealed with Kapton film to avoid air exposure. Profile matching of the powder diffraction data of the as-prepared $NaNi_{1/3}Co_{1/3}Fe_{1/3}O_2$ was performed with Highscore Plus using space group R-3m.


Journal Articles & Patents
Annotated Paragraphs
Annotated Sentences
Grammatical Dependency Parser
asdf... =
Word Embeddings
Desired Text
asdf... =
Word Embeddings
Named Entities
FastText
Recurrent Net
ELMo
Recurrent Net

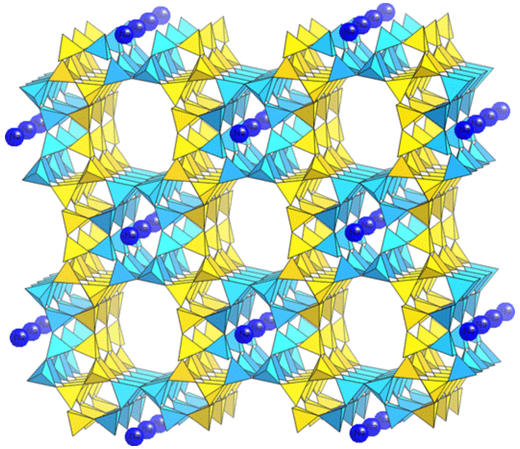
Balance generalized approach with accuracy tailored for specific examples

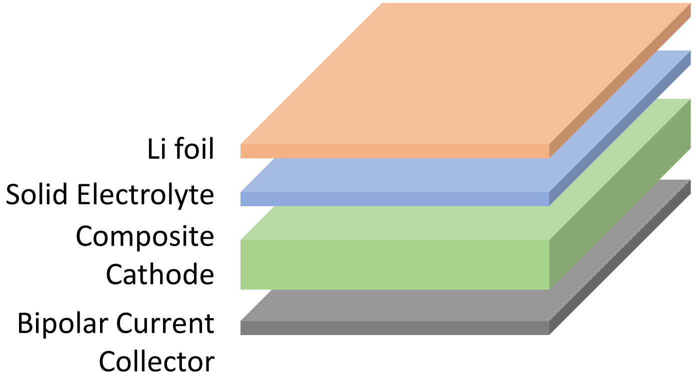
DMSE

Inorganic materials synthesis

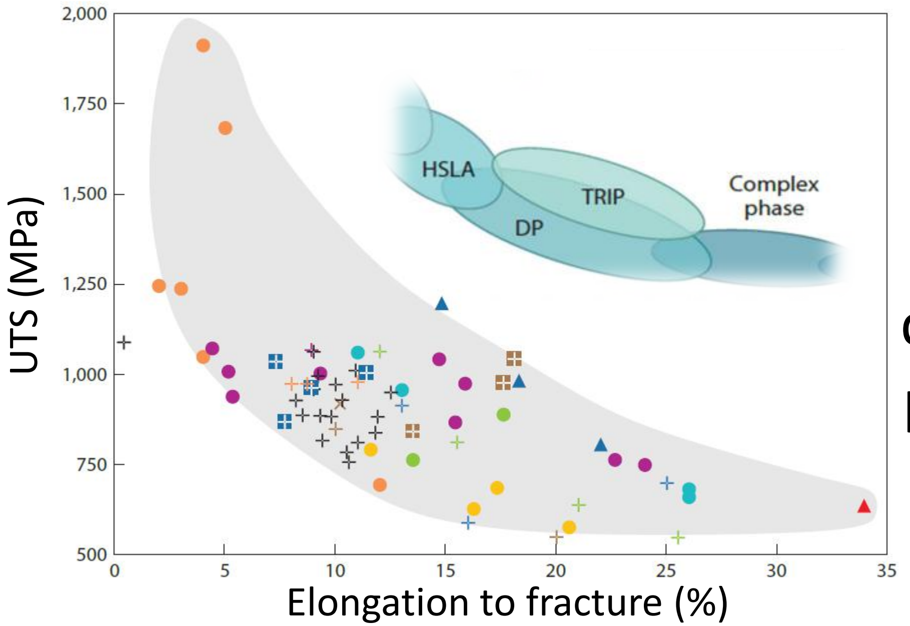


Directing zeolite crystallization



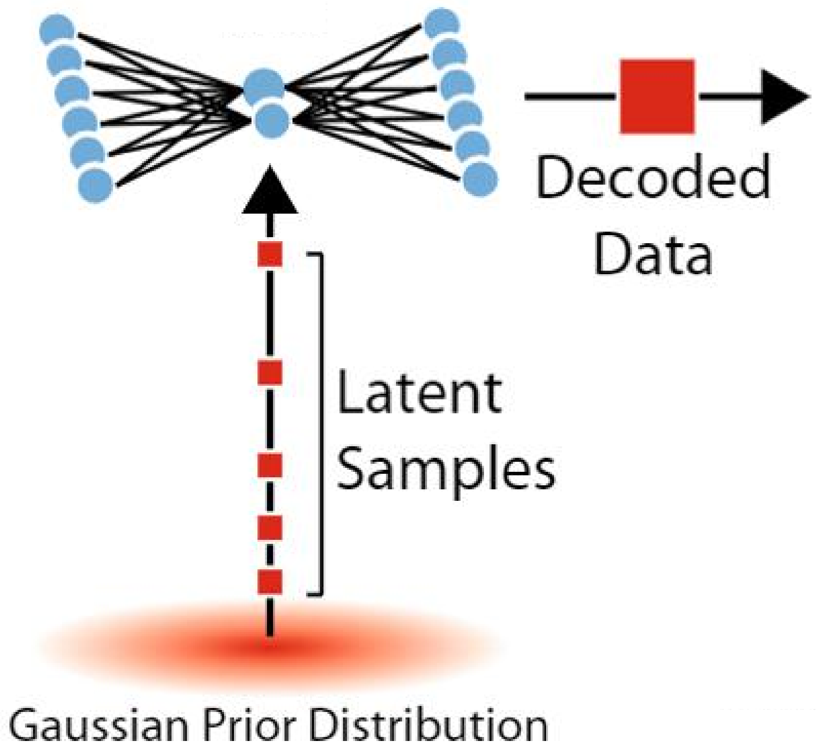


Solid state electrolyte devices



Alloy design and processing

Time-based literature holdouts predict recipes for recently-reported perovskites



Target material	Suggested precursors	Synthesis method
$InWO_3$	In_2O_3+WO_2	Solid state
	$InCl_3$+Na_2WO_4 [1]	Solution phase
$PbMoO_3$	$PbSO_4$+$MoCl_2$	Solution phase
	PbO+MoO_2 [2]	Solid state

Validation includes: reaction enthalpies, commercial availability

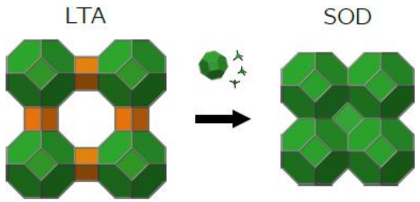
Screening approach: Within 10 attempts; at least 1 feasible route with commercially available precursors

E. Kim et al., under review
[1] J. Kamalakkannan, et al., *World Scientific News,* 2016
[2] H. Takatsu et al., *Physical Review B,* 2017

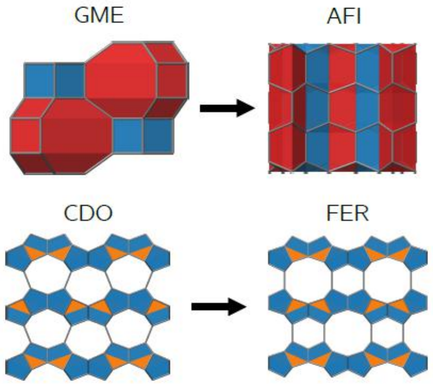
Collaboration with S. Jegelka

Many more zeolites are predicted to be stable than have been realized experimentally

Recrystallization

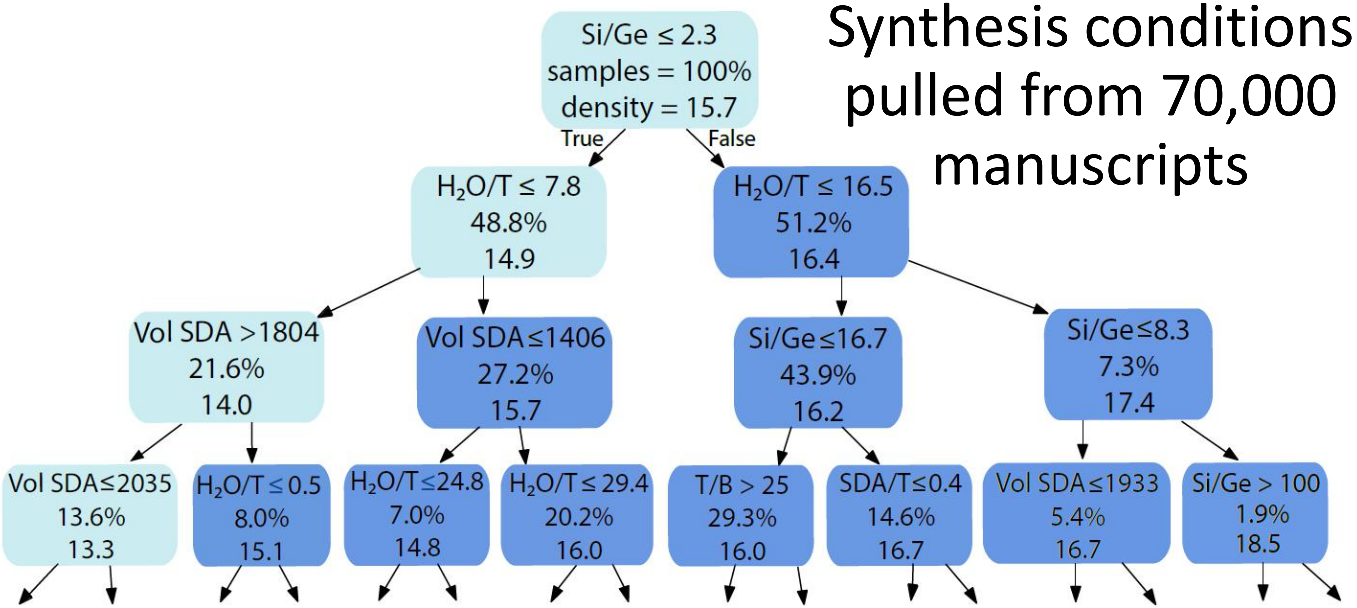


Diffusionless



Applying similarity to 250k zeolites, we found 4k zeolite which are graph isomorphic to known ones.

with Gomez-Bombarelli group



Synthesis conditions pulled from 70,000 manuscripts

Predicting synthesis pathways for low framework density zeolites

Z. Jensen et al., *ACS Central Science*, 2019
Schwalbe-Koda et al *Nature Materials*, 2019

Production in Lab

KEY DRIVERS

- Materials
- Process and equipment
- Heat and mass transport

KEY OUTCOMES

- Performance

Manufacturing at Scale

KEY DRIVERS

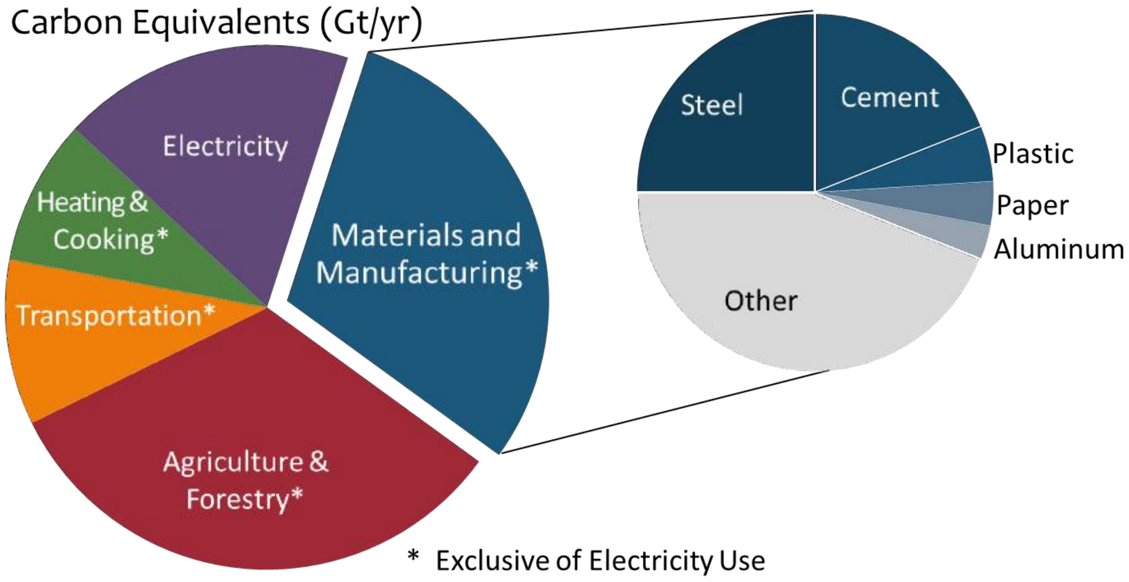
- Materials
- Process and equipment
- Heat and mass transport
- Process rate
- Process yield
- Energy use
- Process knowledgebase
- Infrastructure maintenance

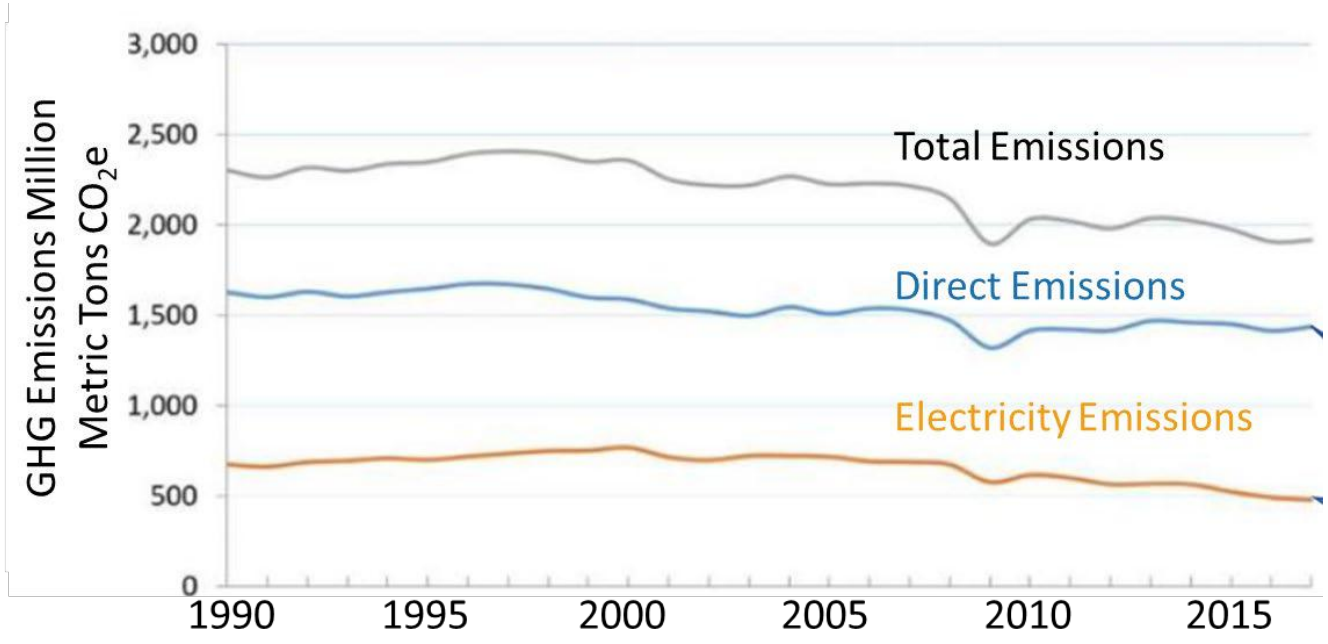
KEY OUTCOMES

- Performance
- Reproducibility
- Production volume
- Production cost

Huang, et al. *Joule* 2018

There are significant opportunities beyond electricity

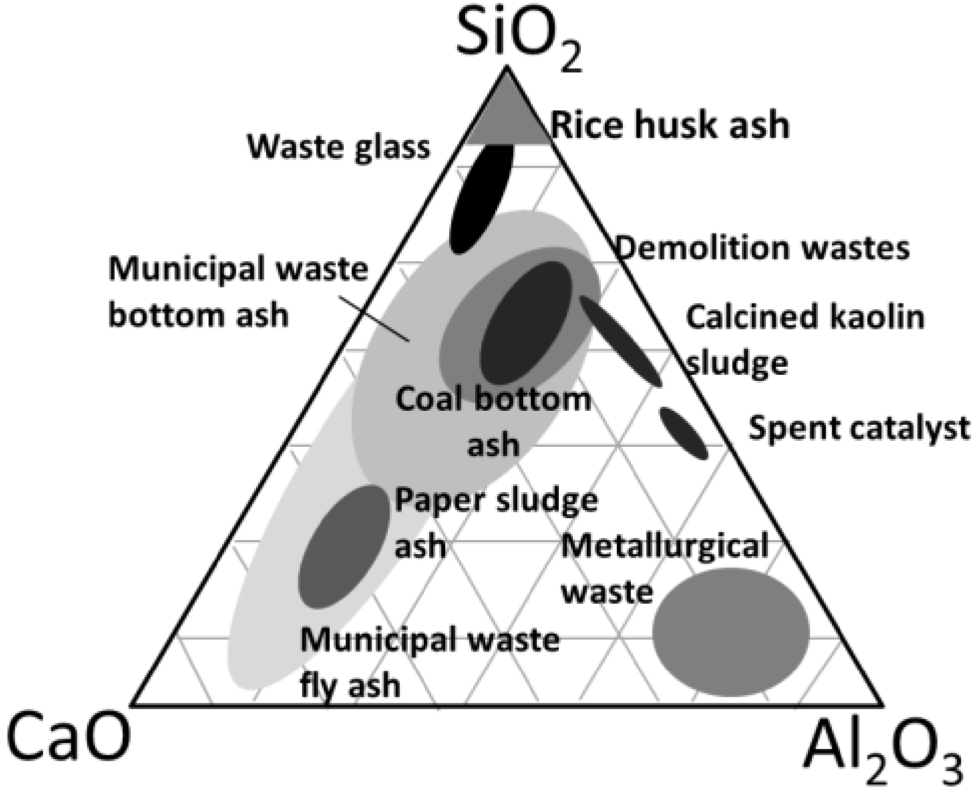


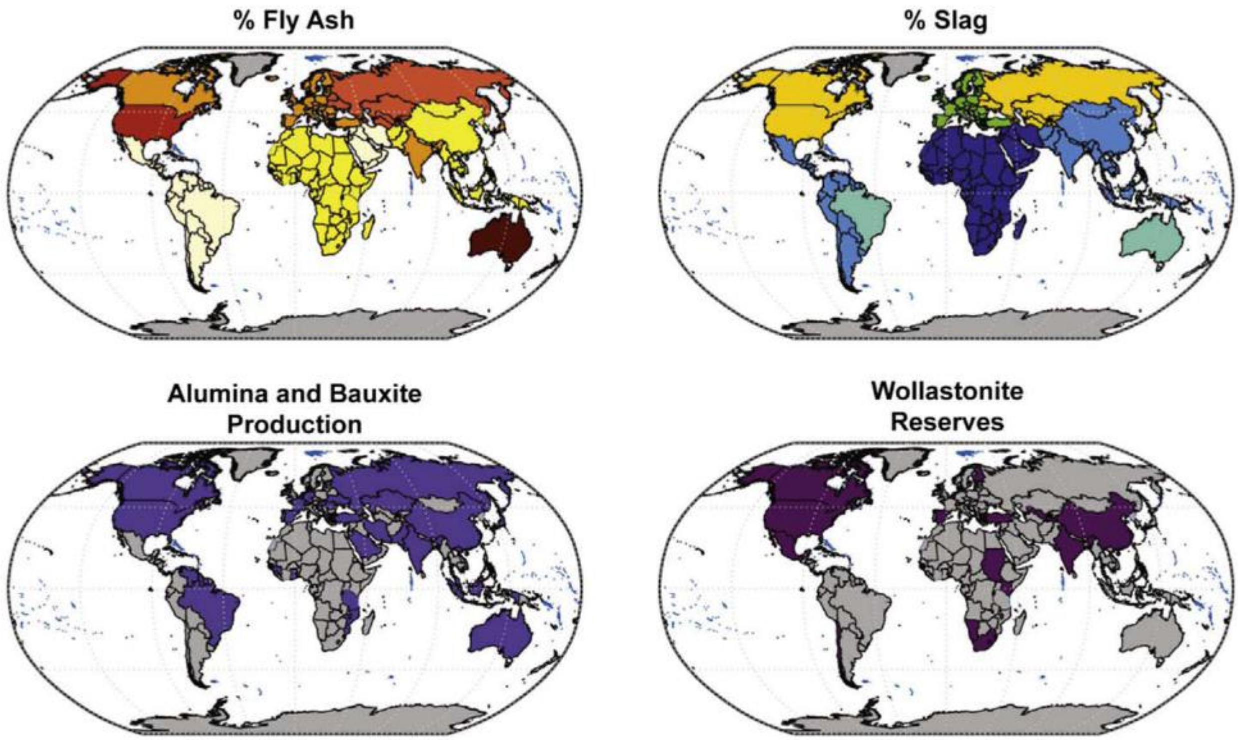


Source: DOE (2014) EPA (2018)

(left figure) Sassoon, R., et al.. *Quantifying the Flow of Exergy and Carbon*. 2009 MRS Spring Meeting
(right figure) Allwood, J., et al., *Options for Achieving a 50% Cut in Industrial Carbon Emissions by 2050*, ES&T, 2010, 44 (6).

Design cements across broad set of wastes, enable sophisticated beneficial use

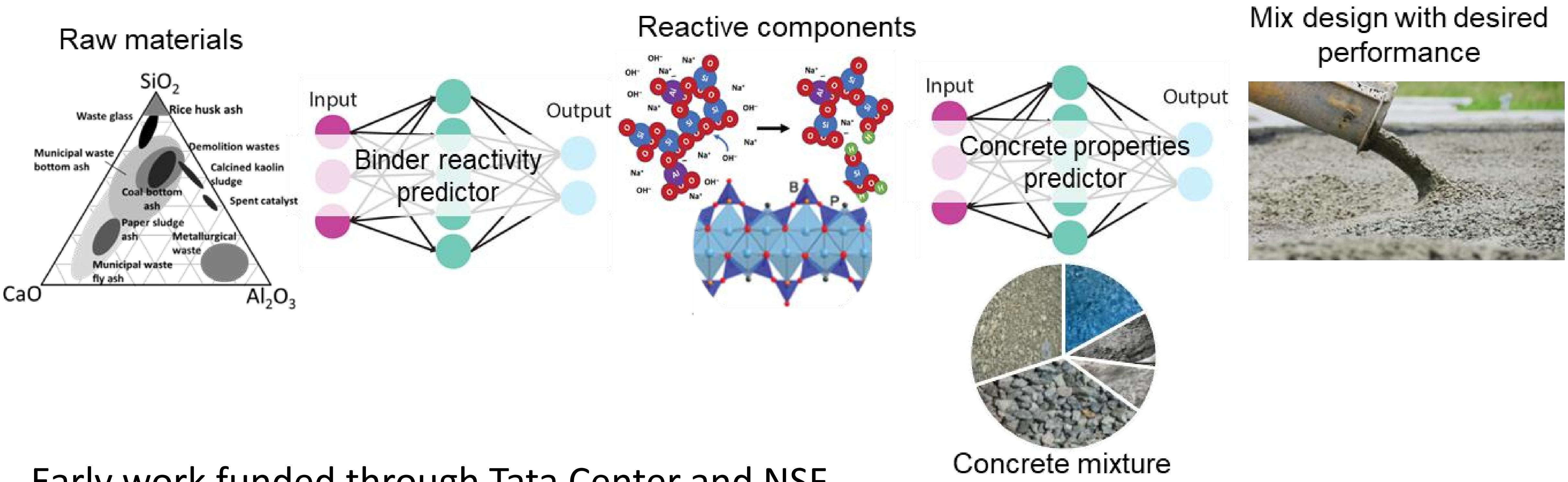




T. Poinot et al., *Resources Conservation and Recycling, 2017*
P. Chaunsali et al. *Cement Concrete Composites*, 2018, 2019

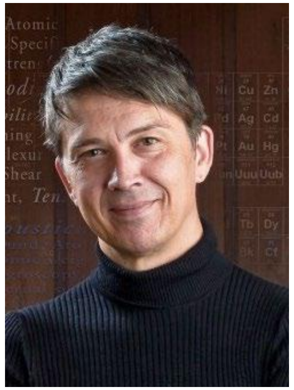
Miller et al., *Cement and Concrete Research,* 2018

Develop low environmental impact concrete mixtures through effective use of waste materials



Early work funded through Tata Center and NSF,
now funded through MIT-IBM Watson AI Laboratory

Thank you



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ITQ (Moliner and Corma)
olivetti.mit.edu; synthesisproject.org