Finding holes in materials

A first step toward better batteries

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Finding holes in materials

Motivation

Problem

Our Solution

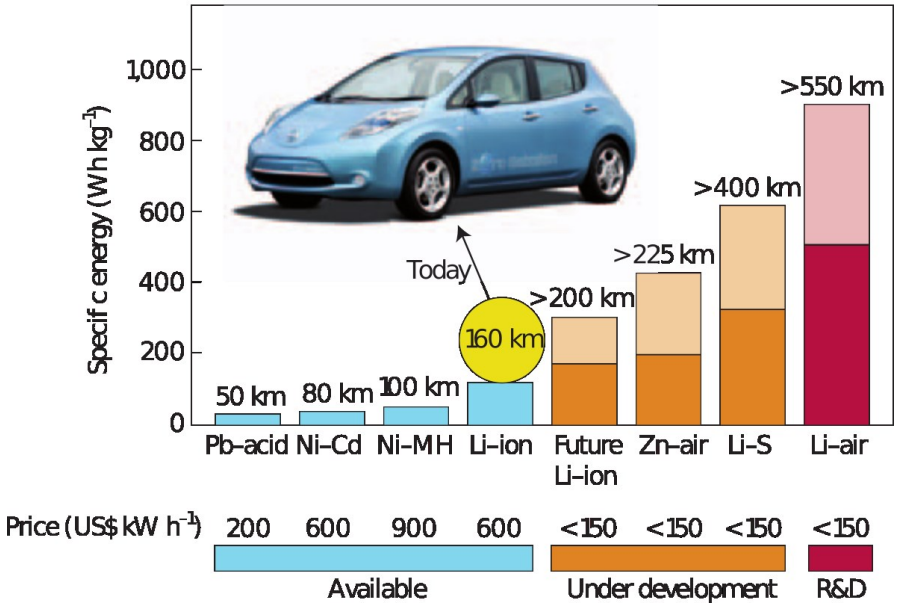
Extra credits

The future of batteries

Battery 500 project

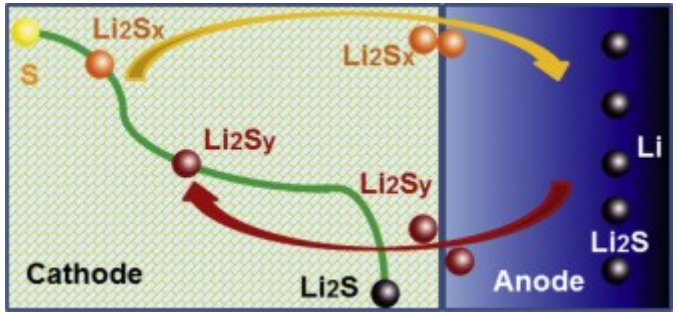
MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH



Practical specific energies for some rechargeable batteries, along with estimated driving distances and pack prices. *Nature Materials* **11**, 19–29 (2012)

The future of batteries



Journal of Power Sources, 253, 263

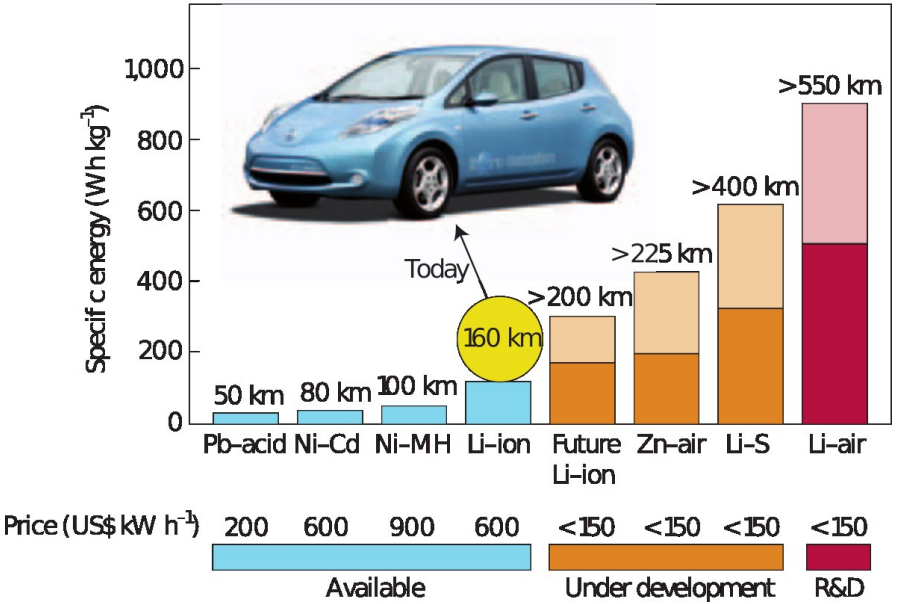


Table 1
The physicochemical properties of some common solvents.

Solvent	FW	d, g cm^{-3} (25 °C)	ε_r (25 °C)	η, mPa s (25 °C)	E_{homo}, eV	E_{lumo}, eV	mp, °C	bp, °C	fp, °C
Ethylene carbonate (EC)	88	1.32 (40 °C)	90 (40 °C)	1.9 (40 °C)	−12.86	1.51	36	238	143
Propylene carbonate (PC)	102	1.2	65	2.5	−12.72	1.52	−49	242	138
Dimethyl carbonate (DMC)	90	1.06	3.1	0.59	−12.85	1.88	5	90	17
Ethyl methyl carbonate (EMC)	104	1.01	3	0.65	−12.71	1.91	−53	108	23
Diethyl carbonate (DEC)	118	0.97	2.8	0.75	−12.59	1.93	−74	127	25

Green Energy & Environment, 1, 18

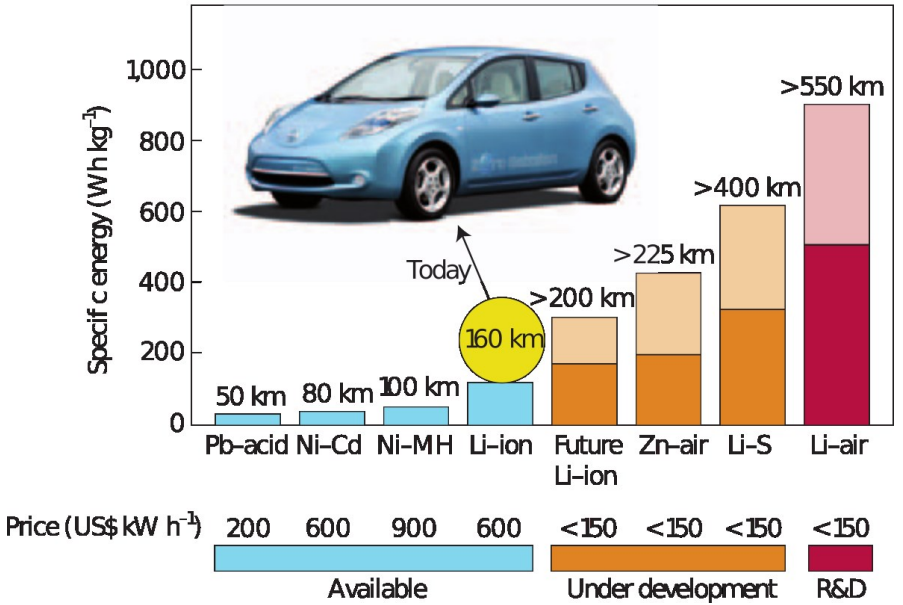
The future of batteries

Issues:

- × Safety
- × Stability
- × Environmental risk

Possible solutions:

- ✓ Ionic liquids
- ✓ Polymers/Gels
- ✓ **Solid-state electrolytes**



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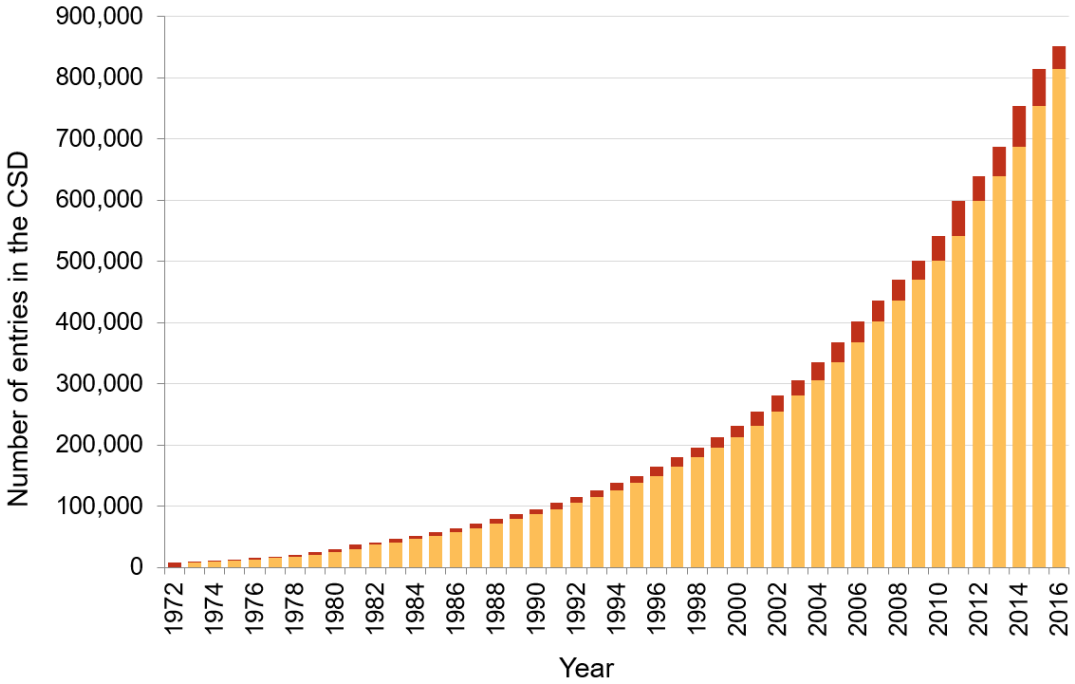
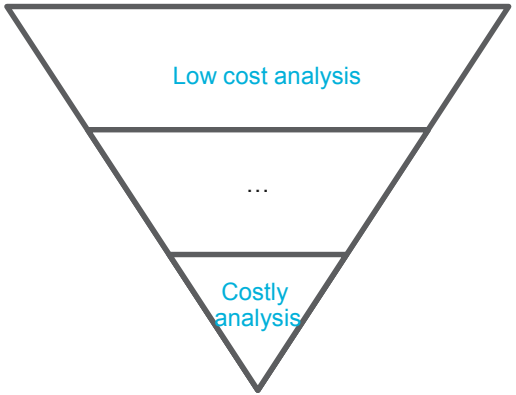
Did we miss it?

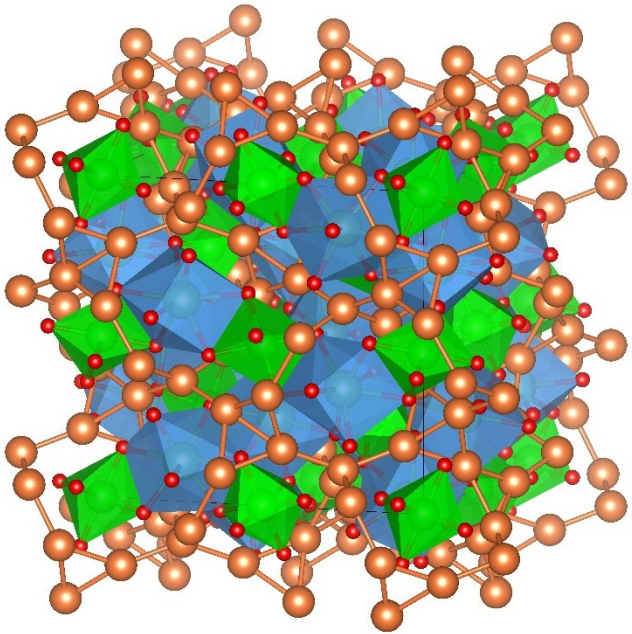


How to find it?

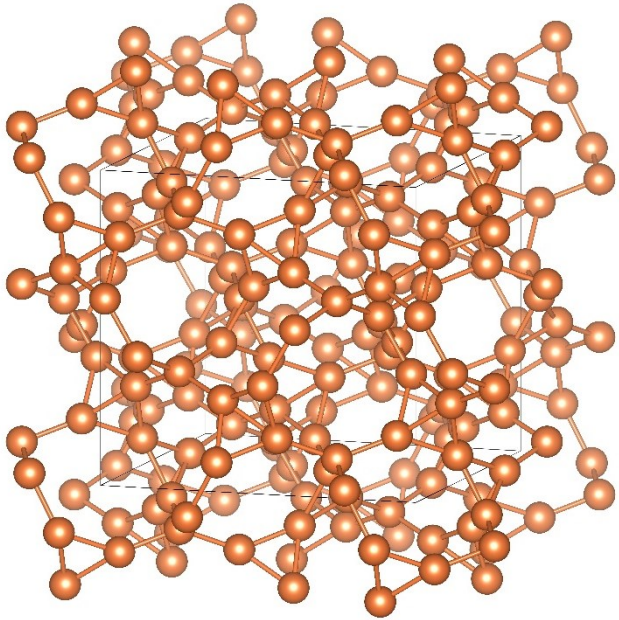


What do we need?

- LLZO: a case study
  - $Li_7La_3Zr_2O_{12}$



- Tetragonal structure at RT with highly connected Li network.



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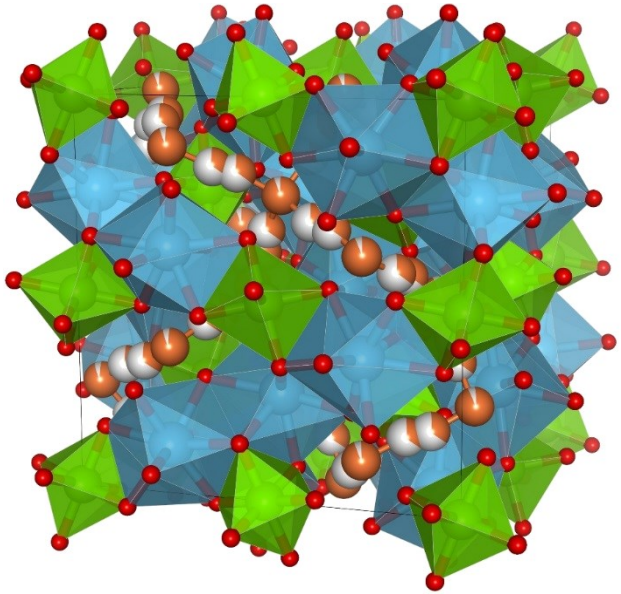

- Cubic structure stabilized by doping among the best known candidates.

- A connected network of sites/holes is no guarantee!
- But a good place to start…

How to measure it

- List of channels, network
- Directionality
- Average/min/max section
- …
- Barrier and potential profile

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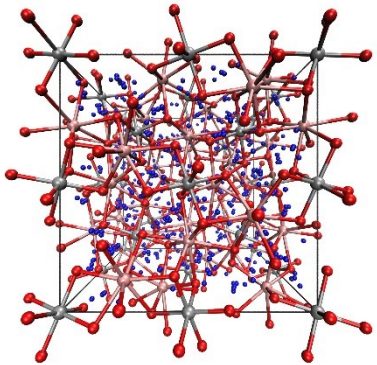
Voronoi diagram



1. Find the vertices

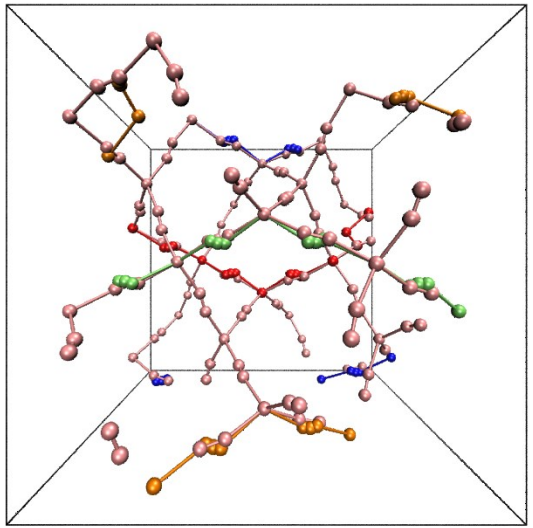
2. Filter

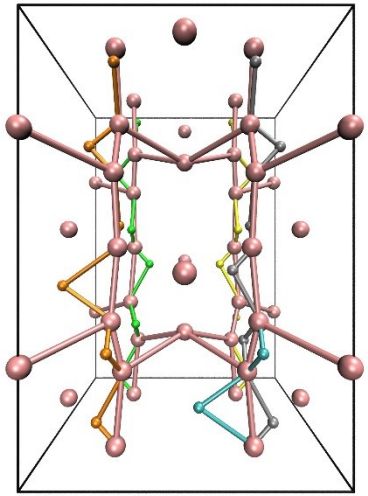
3. Connect

4. Find paths (with/without constraint)

2. Filter based on the ionic radii of the neighbors and the particle size
3. Connect based on the ionic radii of the neighbors and the particle size
4. Constrain to minimum energy path/minimum barriers/…

Voronoi diagram





Getting started

- http://github.com/mottetm/ibm-aim-2016

- 5 structures with conductive properties
- Follow the link for the radii

- Files can be visualized with VESTA

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- Radii depends on:
  - Charge,
  - Coordination (how many neighbors, special arrangement),
  - Spin

- Find the charge and coordination programmatically.

Thank you for your attention

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