TECHNISCHE UNIVERSITÄT BERGAKADEMIE FREIBERG

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Institut Experimentelle Physik

R2R BATTERY

Assessing Al-ion conductors from sulphides and selenides

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Atom	Size	Polarisability	ICSD (Al + X)
O	Very small	none	10,077
S	Quite large	high	641
Se	large	high	153

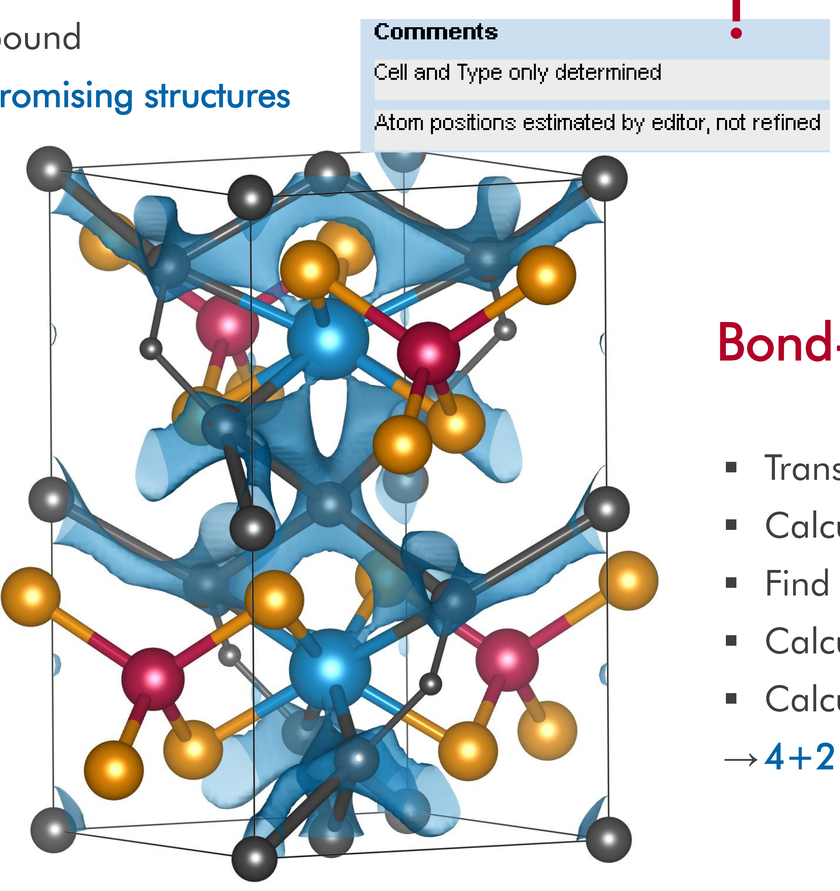
Motivation

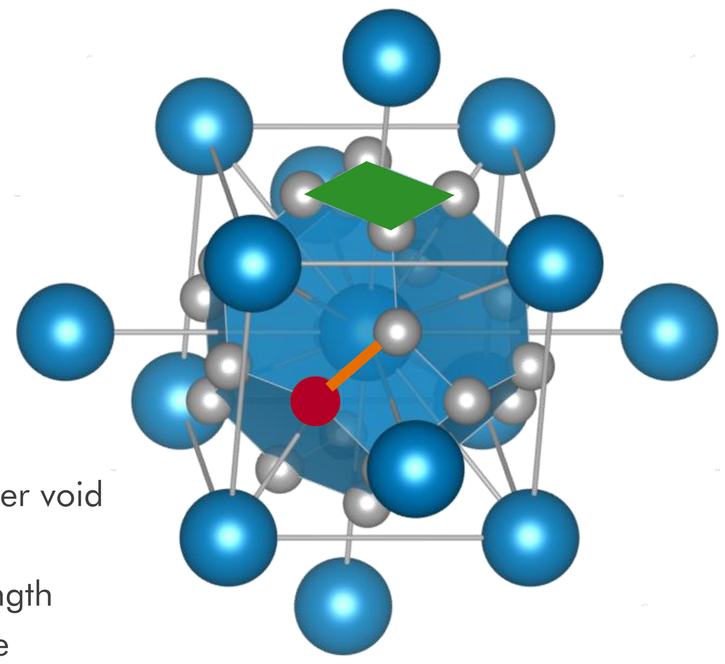
- Electrochemical energy storage: most promising for **sustainable technologies**
- **Aluminium** (Al): high **abundance**, low price, high capacity (trivalent)
- So far no reliable Al^{3+} **conductor/intercalation host** identified
- **CryPhysConcept**: combine **crystallography**, **electrochemistry** and **resource aspects** to create new concepts for electrochemical energy storage
- Ion **diffusion in crystals**: ion jump between two sites (via an intermediate)
- **Shield** high charge of Al^{3+}: find compounds with S/Se (**polarisability/size**)

Voronoi-Dirichlet Partitioning

- **Data mine** reference values from **ICSD**:
  atomic soft sphere radii r_{SD} and crystal chemical data on **Al-S/Al-Se**
- Find most-promising entries from all **Al and S/Se containing compounds**
- Compare all **structural voids** with reference values [1]
  (*c.f.* Meutzner, *Cryst. Res. Technol.* **52**, 1600223 (2017))
- Calculation time: **fraction of a second**
  per compound

→ **37 + 5 promising structures**





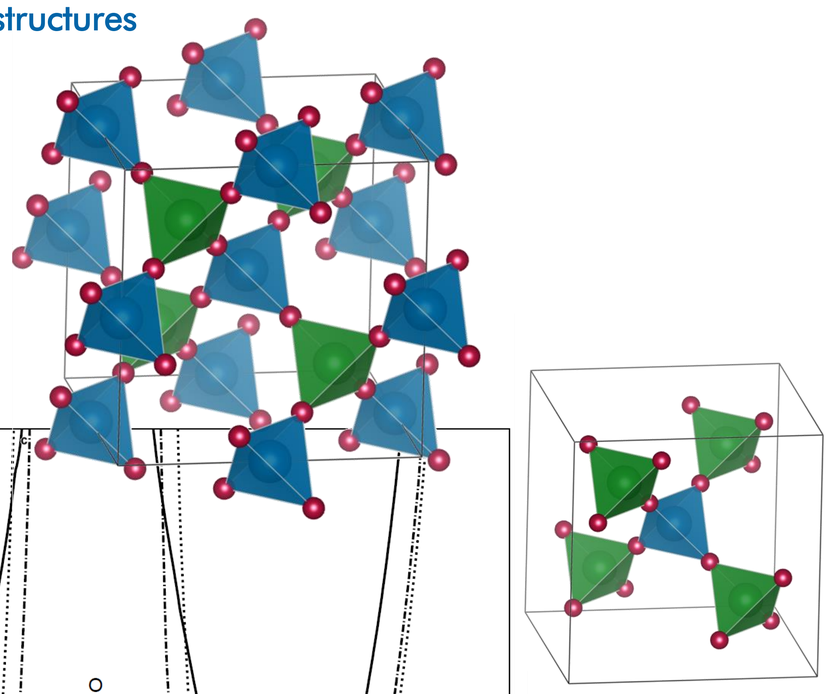
Ionic Conductivity

- **Vertices** — voids
  possible ions to enter void
- **Edges** — channels
- **Faces** — bond strength
- **Volume** — ionic size

Bond-Valence Energy-Landscape

- Translate **bond-valence sum mismatch** into energy [2]
- Calculate for the **whole crystal volume** (resolution of 0.1 Å)
- Find lowest energy barrier → **activation energy** for diffusion
- Calculate for Al^{3+}, S^{2-}/Se^{2-} and all other remaining elements
- Calculation time: **minutes to hours** per compound

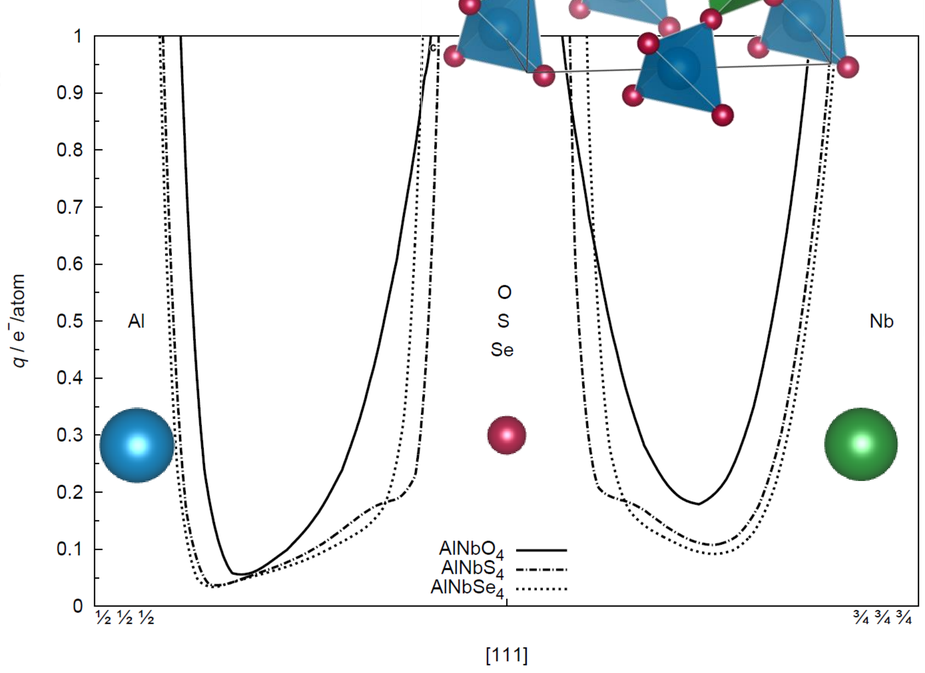
→ **4+2 promising structures**



Density Functional Theory

- Calculate **electronic configuration** *ab initio*
- **Nudged Elastic Bands** (NEB) algorithm calculates energies for all **intermediate steps** between initial and final atomic arrangement [3]
- Each step is **fully electronically relaxed**
- Only done for a very small amount of compound
- Calculation: **hours to days** per compound

→ Work in progress



Summary & Outlook

- Combination of **advantages** into new algorithm
- Applicable for **any sort of ion**
- Efficient in **time and conclusion**
- Synergies bring **development** for each method
- Experimental **proof-of-principle**

→ Full results to be submitted in 2016

[1] Blatov *et al.*: *Acta Crystallogr. B* **62**, 1010–1018 (2006).

[2] Adams *et al.*: *Physica Status Solidi A* **208**, 1746 (2011).

[3] Kresse *et al.*: *Phys. Rev. B* **54**, 11169 (1996).

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