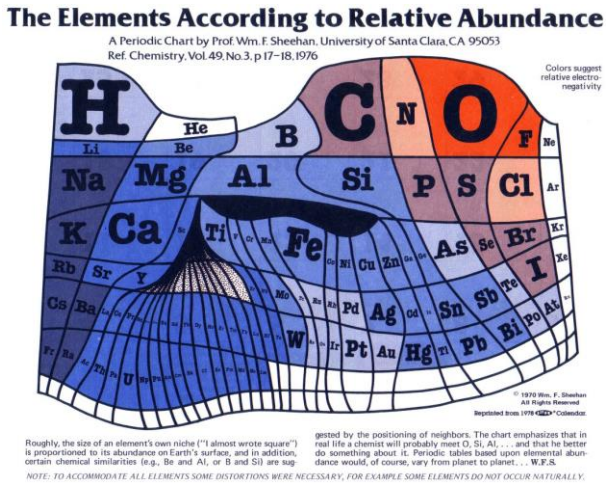
Computer modelling studies of electrolyte materials for solid-state sodium batteries

Solid-state electrolytes

- ✓ Safety
- ✓ Stability
- ✓ Energy density
- × Bulk conductivity
- × Grain boundaries
- × Interfaces

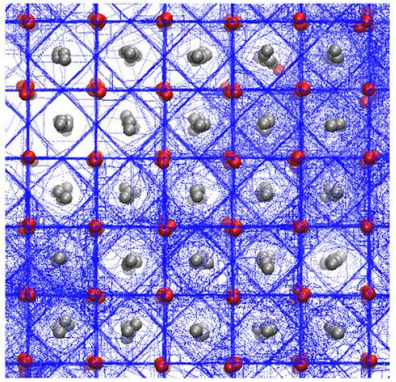
Sodium

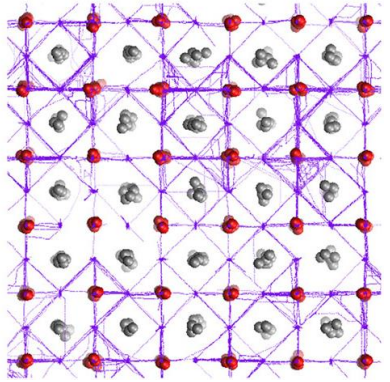
- ✓ Abundance
- × Energy density



Computational modelling

- Molecular dynamics based on atomistic potentials
- Mean square displacement → conductivity, activation
- Time averaged densities → trajectory plots





References:

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2. J. A. Dawson *et al.*, *J Am Chem Soc.*, 2018, **122**, 42, 23978–23984