Atomistic doping effects in the Na_3OCl antiperovskite electrolyte for solid-state batteries

Ben Goldmann, Matt Clarke, James Dawson and Saiful Islam

EPSRC Centre for Doctoral Training, Centre for Sustainable and Circular Technologies, University of Bath, BA2 7AY, UK
email: bag27@bath.ac.uk, web: www.csct.ac.uk

Background: Solid-State Batteries

Advantages:
- stability
- safety
- energy density

Issues:
- ↓ ionic conductivity
- dopant effects
- interfaces
- grain boundaries

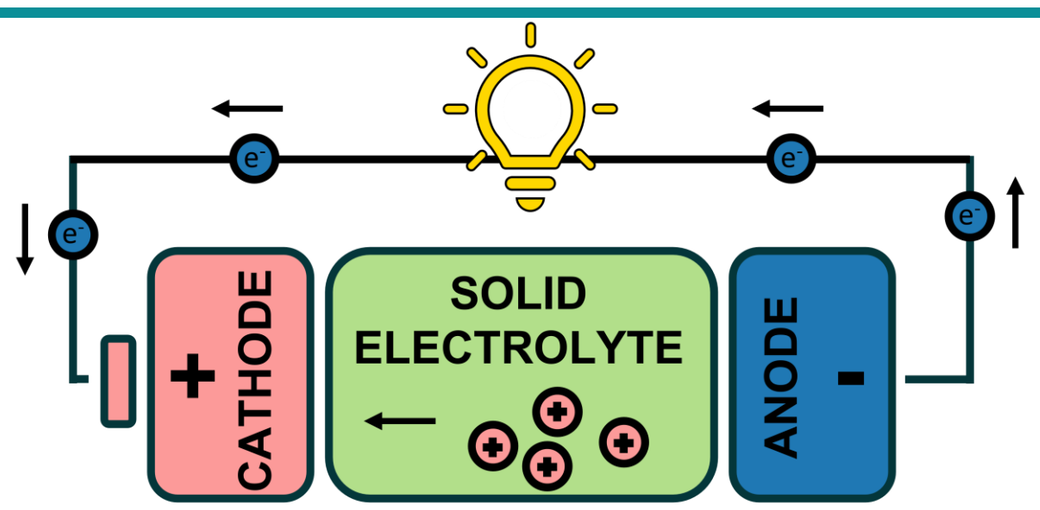

Fig. 1 – Solid-state battery during discharge.

Sodium vs. Lithium

Sodium batteries:
- abundance
- cost
- sustainability
- for renewables

Lithium batteries:
- energy density
- for portable electronics

Project Aims

Atomistic modelling of Na_3OCl solid electrolyte:
- intrinsic defect chemistry
- cation doping to increase defect concentration
- Na-ion conduction
- defect clustering

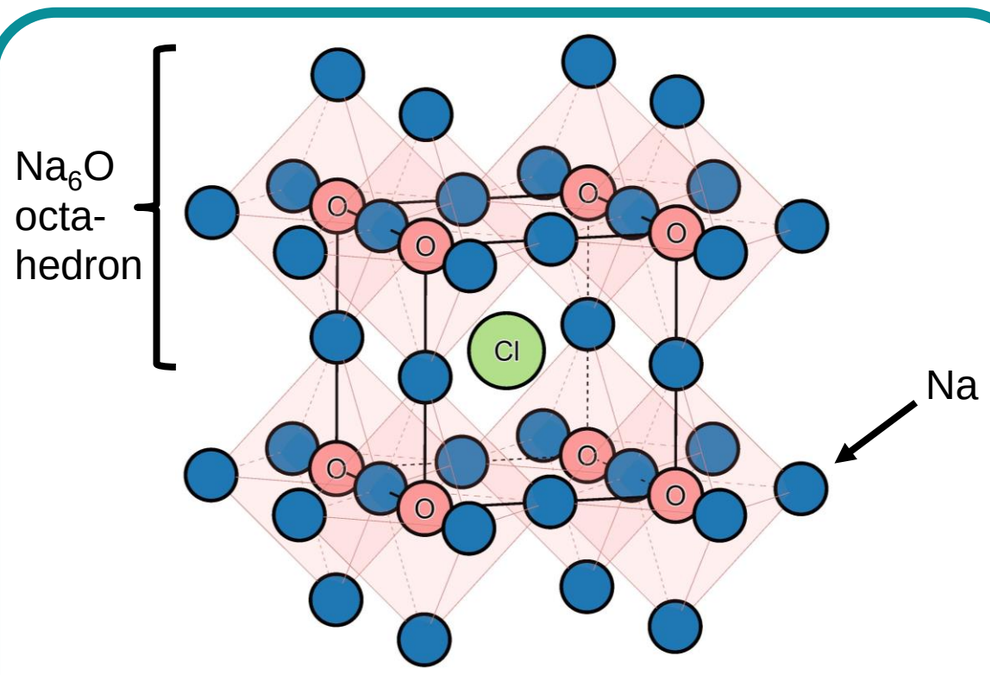

Fig. 2 – The antiperovskite Na_3OCl structure.

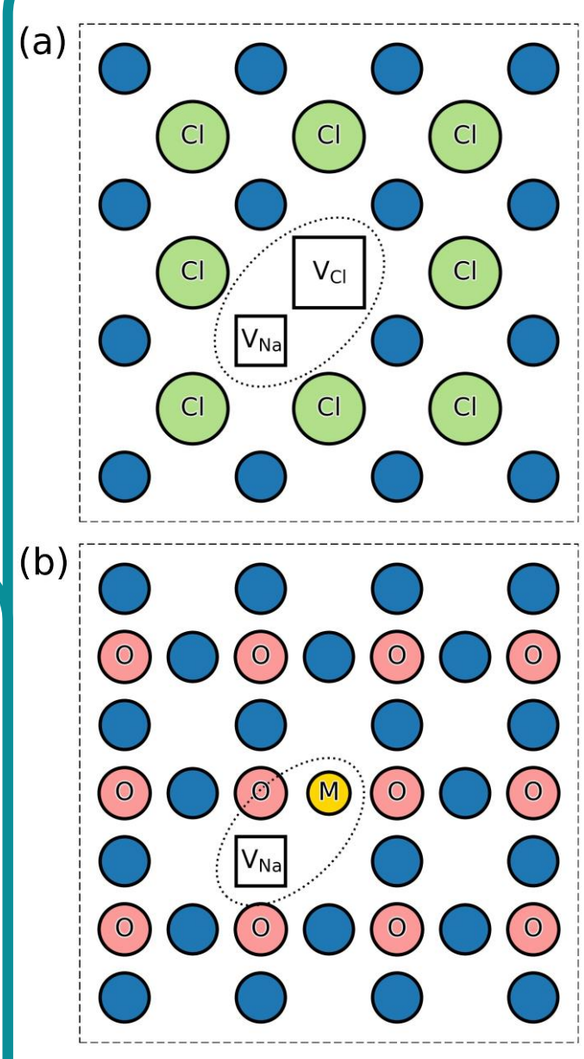

Fig. 3 – Clustering of (a) intrinsic defects in undoped and (b) introduced defects in doped Na_3OCl.

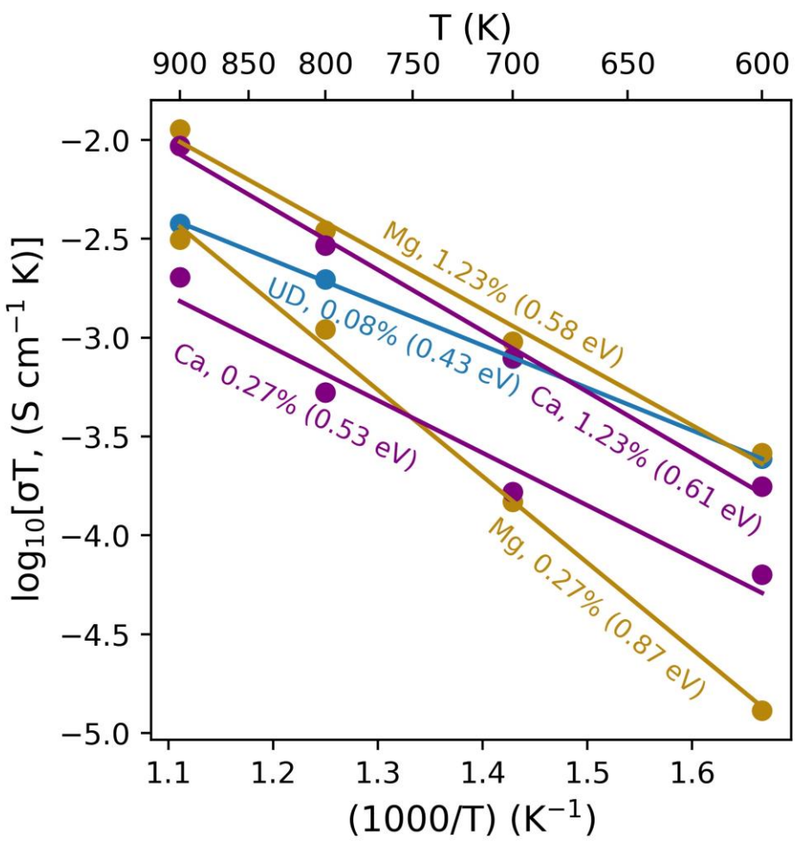

Fig. 4 – Temperature-dependent Na^+ conductivities for Mg- and Ca-doped Na_3OCl.

Modelling doping and ion conduction

- Increased defect clustering in doped material
- Ionic migration limited in doped material at lower Ts
- Higher dopant conc. → increased conductivity

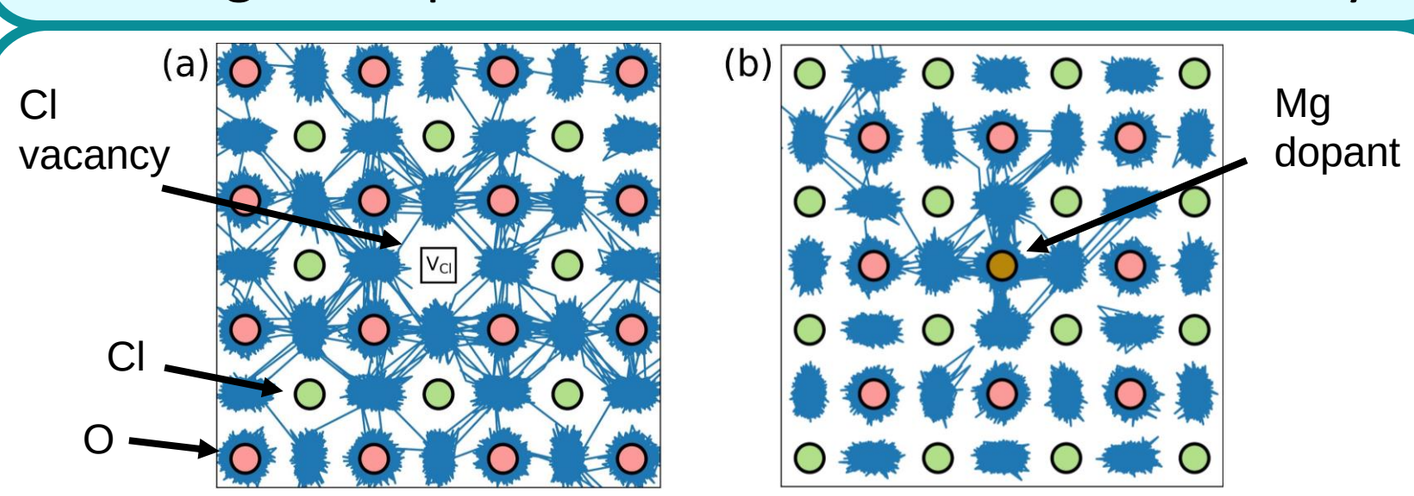

Fig. 5 – Na ion trajectories (blue) in (a) undoped and (b) doped Na_3OCl.