Atomic-scale investigation of doping effects in the anti-perovskite Na_3OCl sodium-ion battery material

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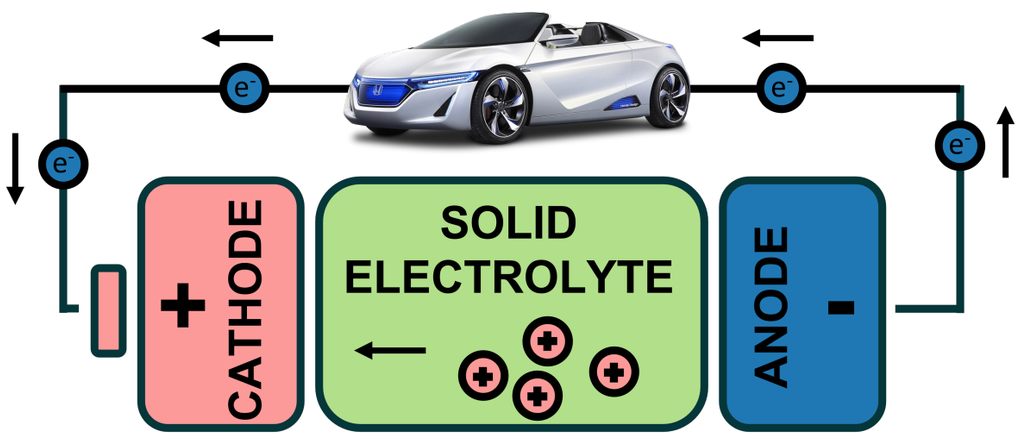
NEXT GENERATION LI-ION CATHODE MATERIALS

Solid-state batteries

Advantages:
- stability
- safety
- energy density

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



Sodium vs. Lithium

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

Lithium batteries:
- energy density
- for portable electronics and electric vehicles

Project aims

Atomistic modelling of Na_3OCl solid electrolyte to gain insight into:
- cation doping to increase relevant defect concentration
- Na-ion conduction mechanism and performance

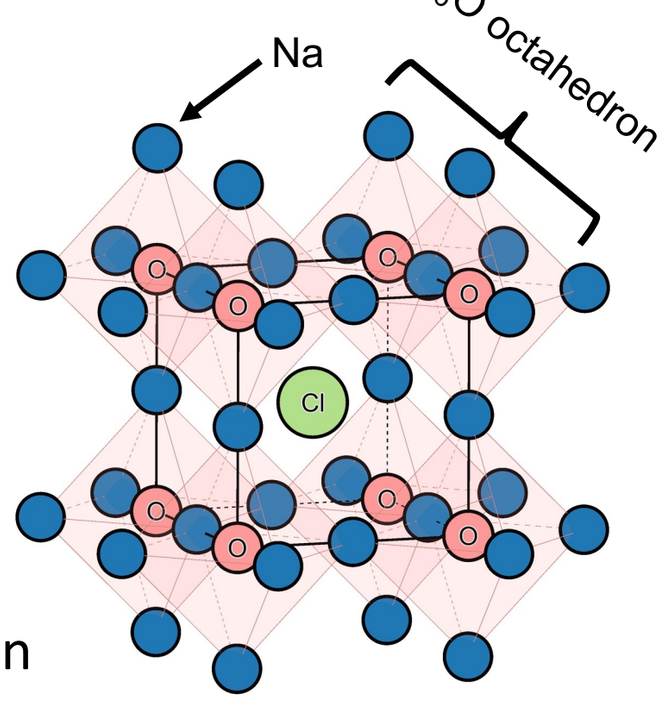


Fig. 1 – The anti-perovskite Na_3OCl structure.

Doping and ion conduction

- Na-ion conduction via vacancy migration along curved pathway at octahedral edges
- Aliovalent doping to induce 1.2% Na-vacancy conc. → increased ionic conductivity

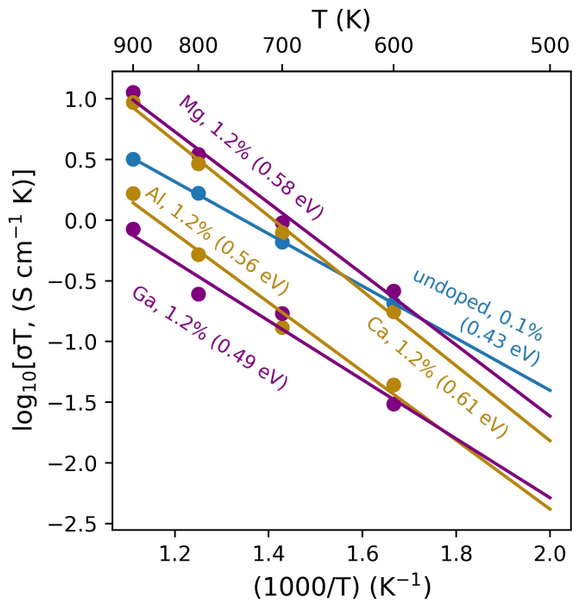


Fig. 2 – Temperature-dependent Na^+ conductivities doped Na_3OCl with 1.2% vacancy concentration.

Clustering effects

- Increased defect clustering in doped materials compared to undoped
- Leads to higher E_a of Na-ion migration

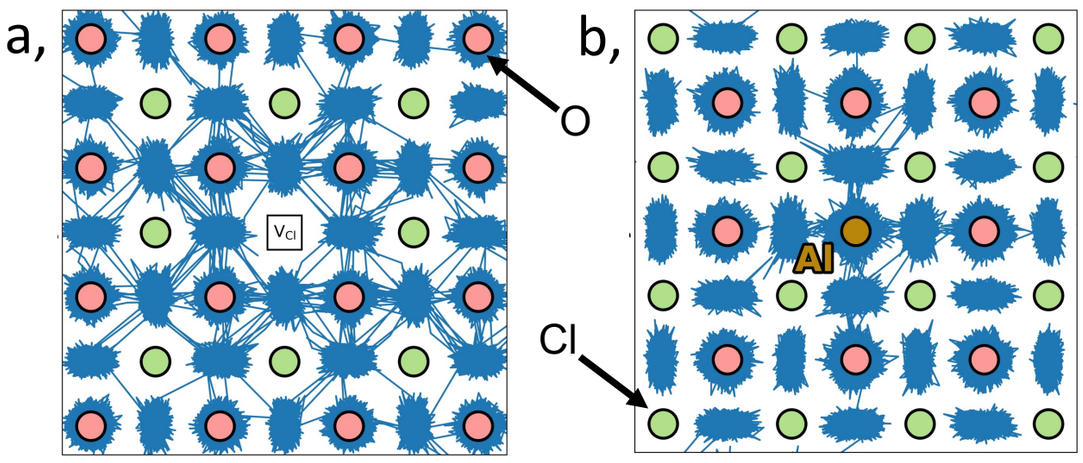
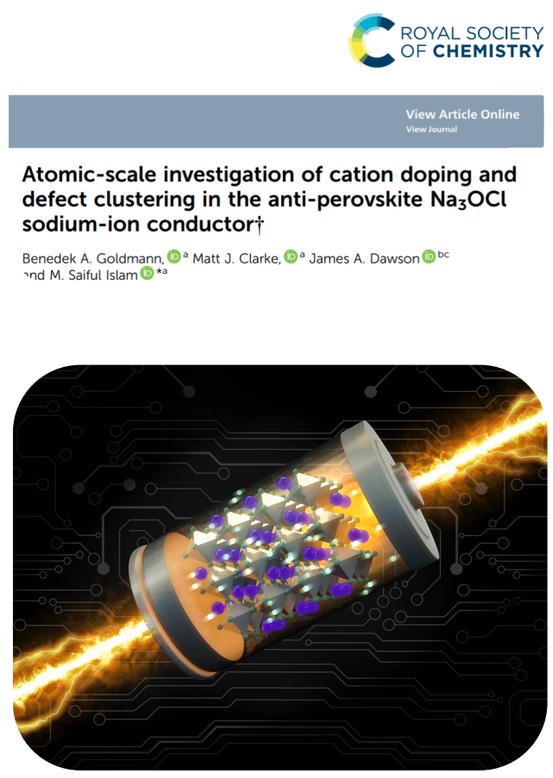


Fig. 3 – Na ion trajectories (blue) in (a) undoped and (b) Al-doped Na_3OCl.

Conclusions and publication

- Atomistic model reproduces Na_3OCl structure accurately
- Favourable dopants include Mg^{2+}, Ca^{2+}, Al^{3+} and Ga^{3+}
- Smallest clustering effect and highest conductivity with Mg^{2+} dopant at 1.2% vacancy conc.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