

# Atomic-scale investigation of doping effects in the anti-perovskite $\text{Na}_3\text{OCl}$ sodium-ion battery material



UNIVERSITY OF  
**BATH**



Centre for **Sustainable  
& Circular** Technologies



THE FARADAY  
INSTITUTION

CATMAT

NEXT GENERATION LI-ION CATHODE MATERIALS

Ben Goldmann, Matt Clarke, James Dawson and Saiful Islam

Department of Chemistry, University of Bath, BA2 7AY, UK  
email: bag27@bath.ac.uk, web: www.csct.ac.uk

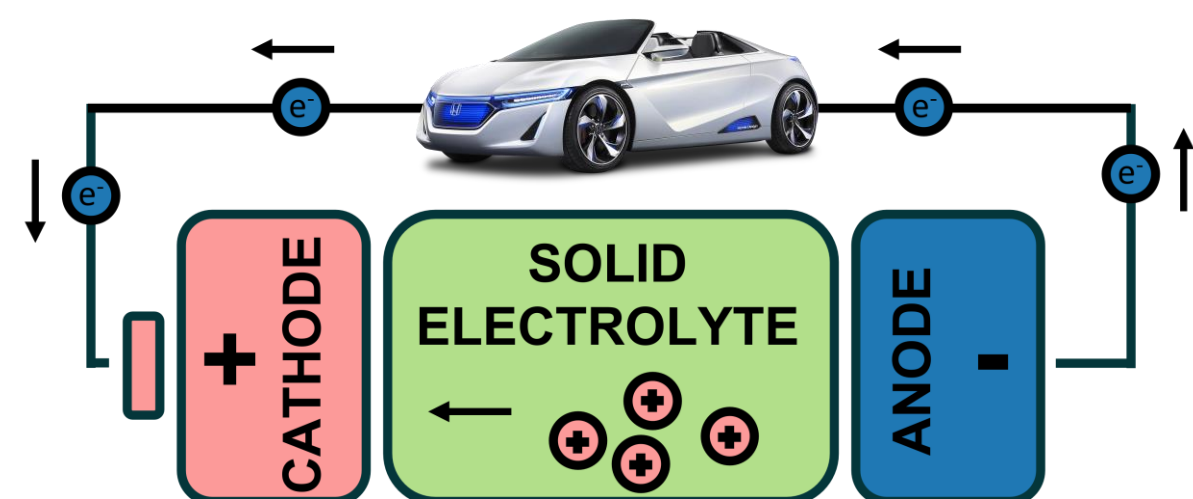
## Solid-State Batteries

### 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 $\text{Na}_3\text{OCl}$ solid electrolyte to gain insight into:

- cation doping to increase relevant defect concentration
- Na-ion conduction mechanism and performance

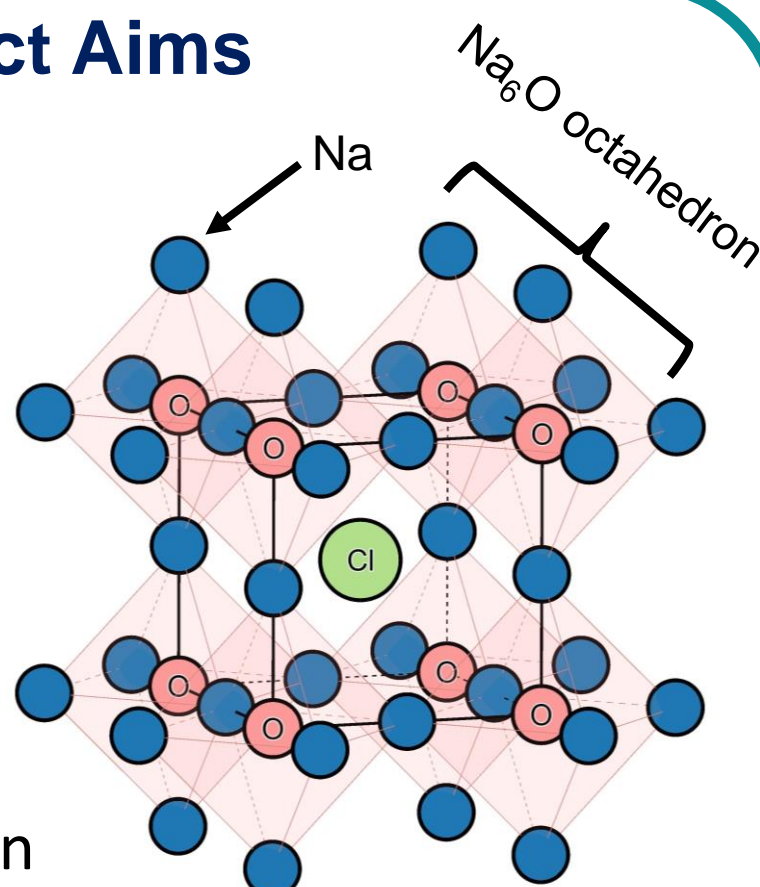


Fig. 1 – The anti-perovskite  $\text{Na}_3\text{OCl}$  structure.

## 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

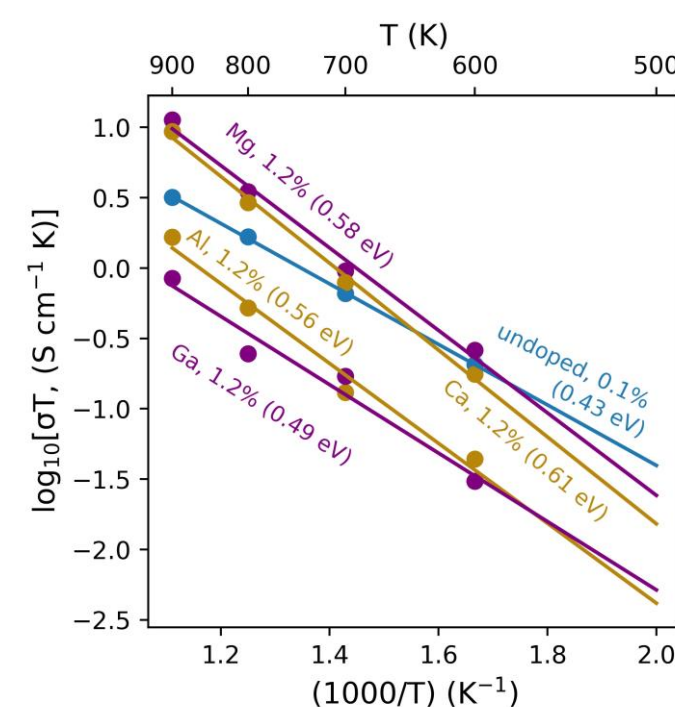


Fig. 2 – Temperature-dependent  $\text{Na}^+$  conductivities doped  $\text{Na}_3\text{OCl}$  with 1.2% vacancy concentration.

## Clustering effects

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

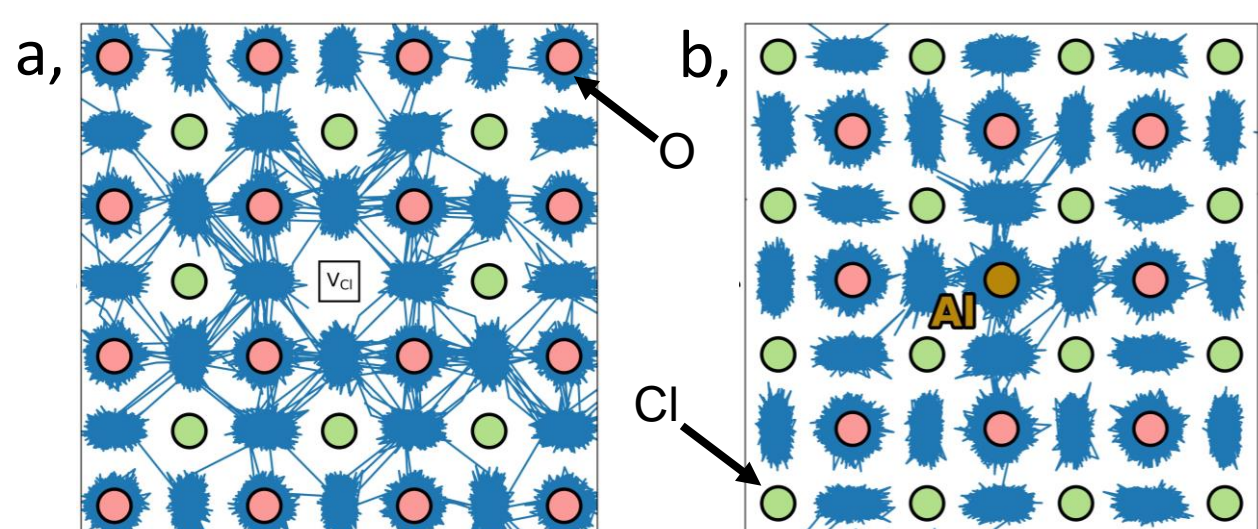


Fig. 3 – Na ion trajectories (blue) in (a) undoped and (b) Al-doped  $\text{Na}_3\text{OCl}$ .

## Conclusions and publication

- Atomistic model reproduces  $\text{Na}_3\text{OCl}$  structure accurately
- Favourable dopants include  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Al}^{3+}$  and  $\text{Ga}^{3+}$
- Smallest clustering effect and highest conductivity with  $\text{Mg}^{2+}$  dopant at 1.2% vacancy conc.



View Article Online  
View Journal

Atomic-scale investigation of cation doping and defect clustering in the anti-perovskite  $\text{Na}_3\text{OCl}$  sodium-ion conductor†

Benedek A. Goldmann, Matt J. Clarke, James A. Dawson and M. Saiful Islam

