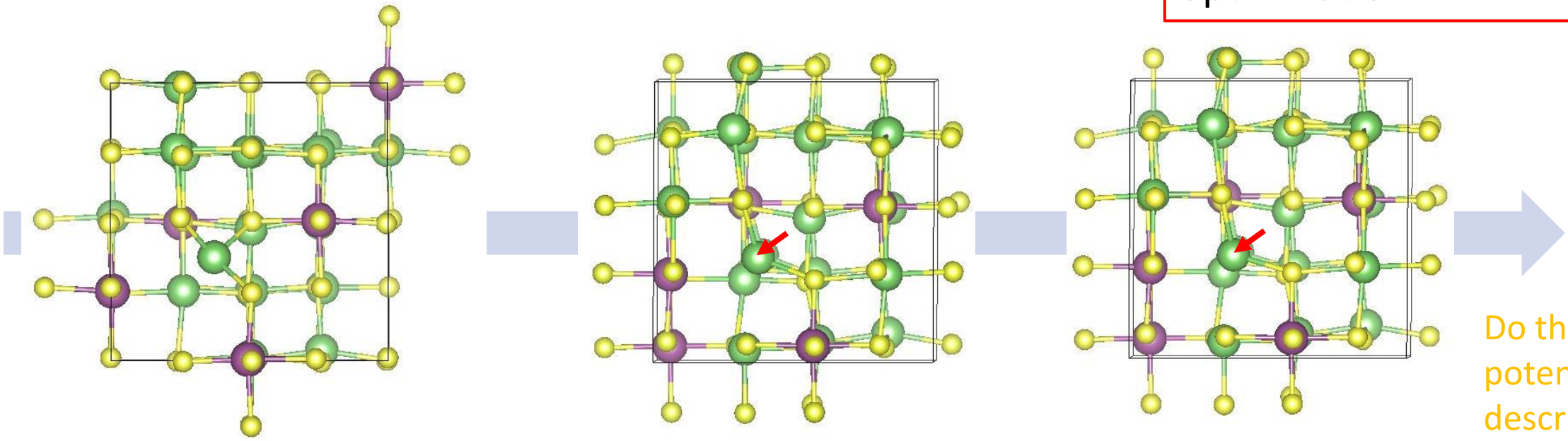
Structural modelling of $Li_2Sc_{2/3}Cl_4$

- Li-Cl, Li-Li potentials used from previous studies
- Sc-Cl potentials fitted to $ScCl_3$

	Exp.	Comp.
a	10.404	10.504
α	90.0	90.3

Movement of Li from 8a tetrahedral to 16c octahedral at 0K optimization



Li Sc Cl

initial

after 100 cycles

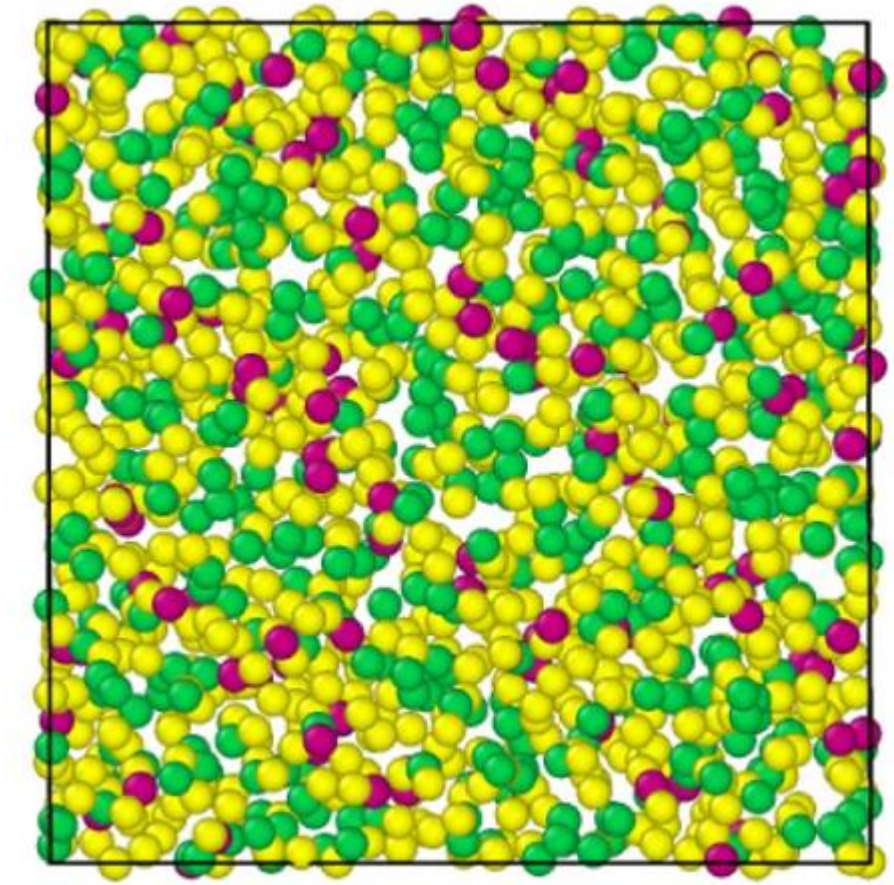
final
(after 659 cycles)

Do the potentials describe the system accurately?

MD simulations

- 2ns
- 1,500 ions
- T = 300 K, 600 K, 900 K

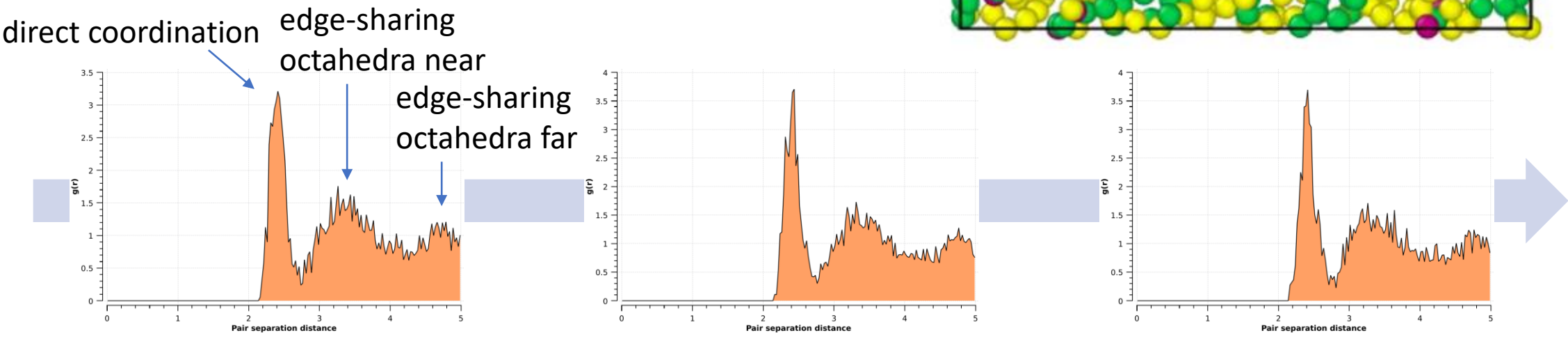
RDFs for the Sc-Cl interactions suggest structural stability, but a dynamic nature



Li

Sc

Cl

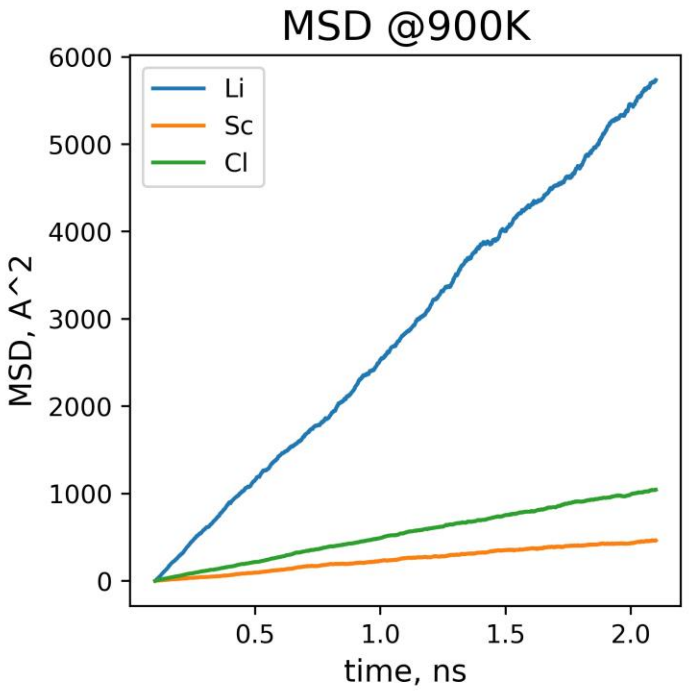


0 ns

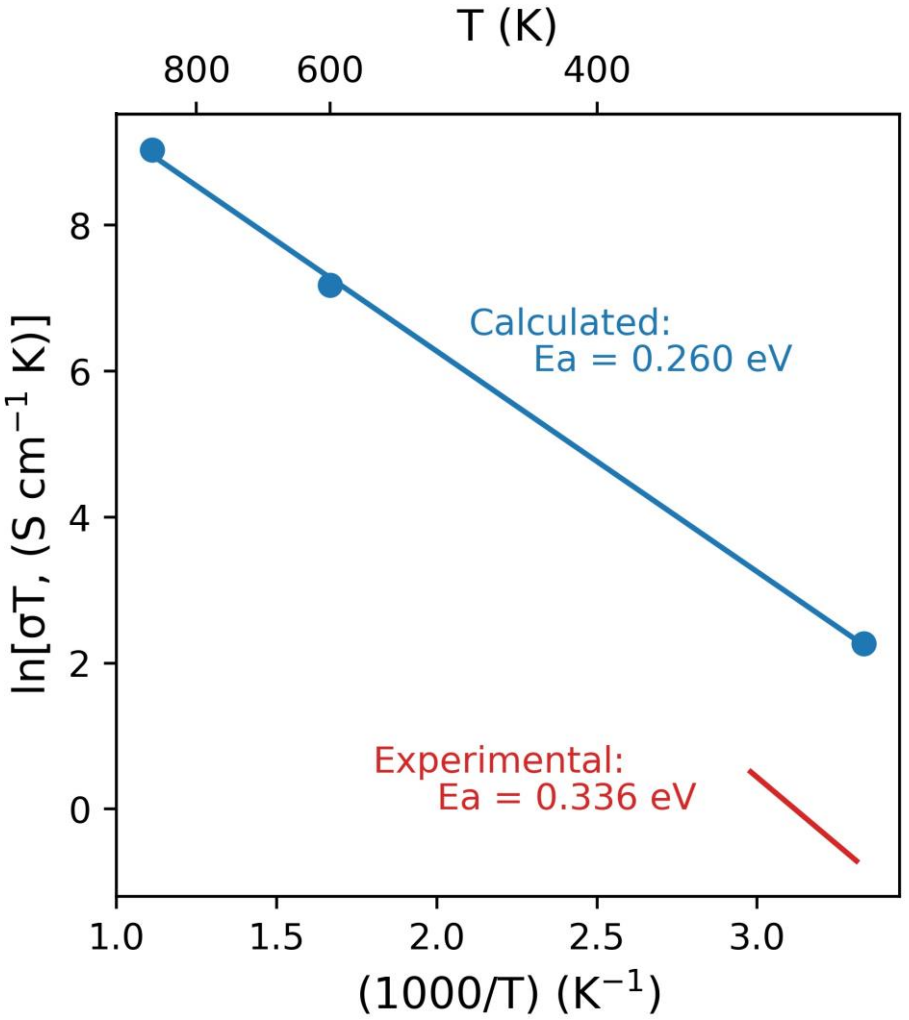
1 ns

2 ns

MD: Li-ion conductivity



Atom	Wyckoff site	U_{iso} (Å^2)
Li1 tet	8a	0.025
Li2 oct	16c	0.038
Li3 tet	48f	0.025
Li4 oct	16d	0.0029
Sc1	16d	0.0029
Cl1	32e	0.0208



Do the potentials describe the system accurately?

RT Conductivity:

- Experimental: 1.5 mS/cm
- Computational: 32.3 mS/cm

Machine Learning (ML)

- Development of ML potentials based on DFT for more accurate modelling of the system
- Investigate 8a tetrahedral vs. 16c octahedral phenomenon to confirm lowest-energy structure using ML potentials
- MD calculations using ML potentials to better understand the inconsistency between experimental and calculated conductivities