

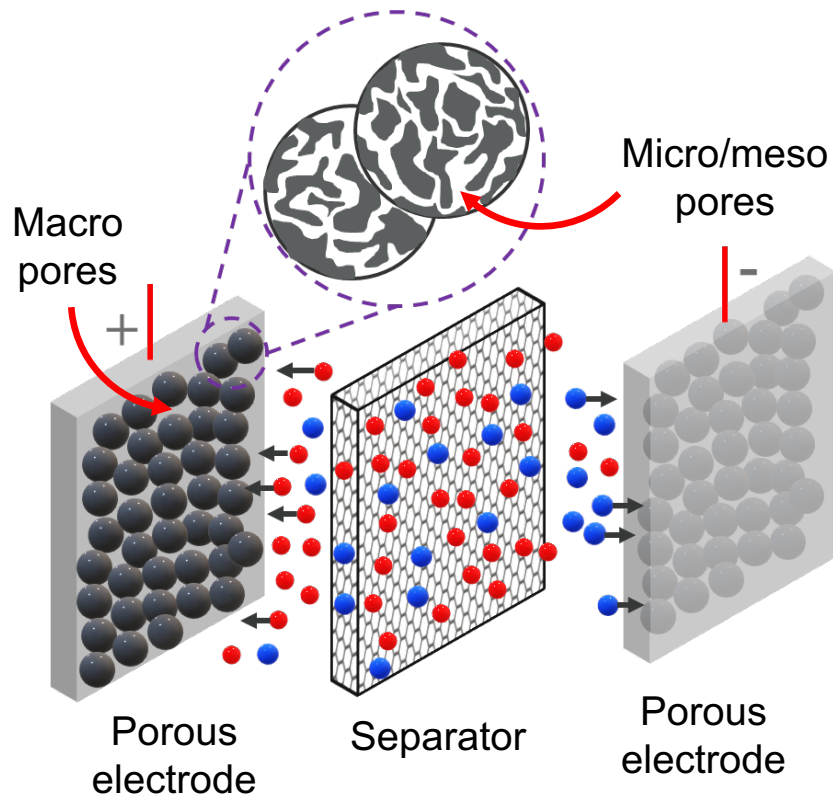
# Molecular dynamics simulations of a supercapacitor with ionic liquid electrolytes

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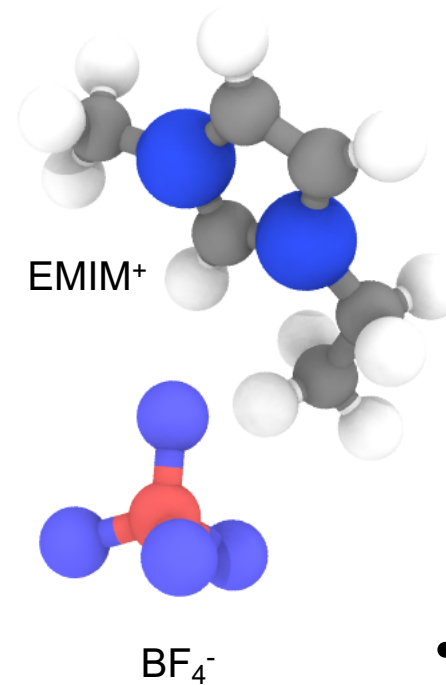


# Supercapacitors (SCs) / Ionic liquids (ILs)

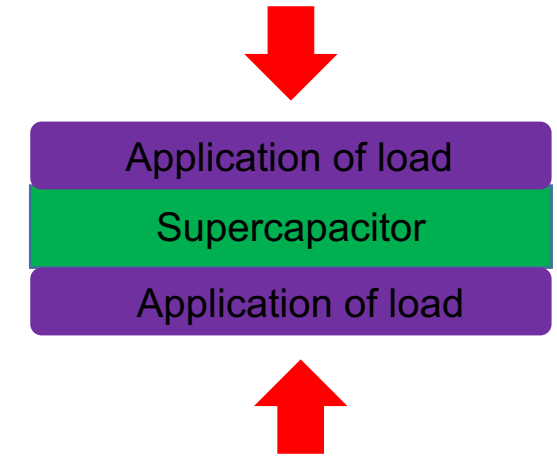
*Supercapacitor*



*Ionic liquid*



*Ionic liquid SCs under loads*

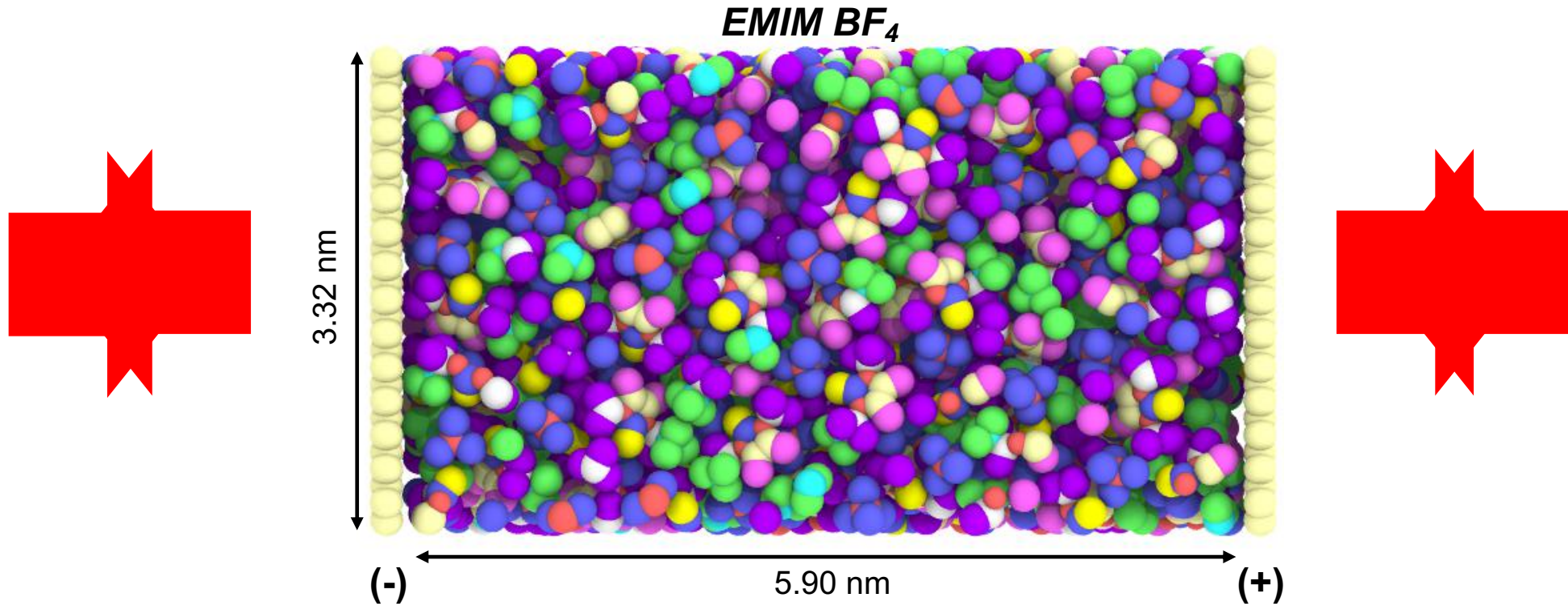


$$E = \frac{1}{2} CV^2$$

- **Flexible SCs/ SCs under load**
- Electrolyte **displacement**
- **Wettability**
- Porous structure **distortion**

Li et al., *ACS Nano*, 2010; Hu et al., Gourdin et al., *J. Power Sources*, 2011, 2012; *Chem. Commun.*, 2018; Moon et al., *Chem. Eng. J.*, 2020

# Structure and method for MD

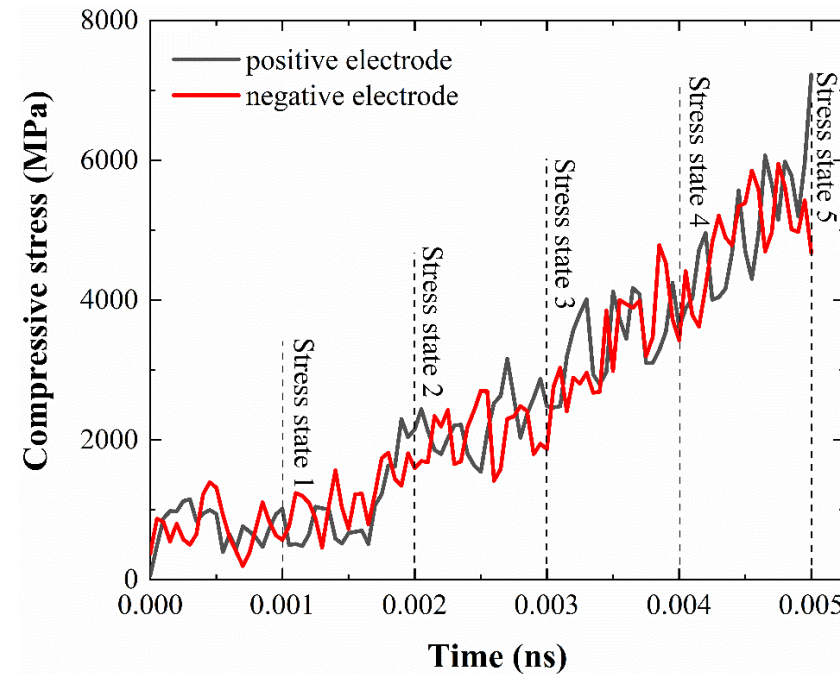
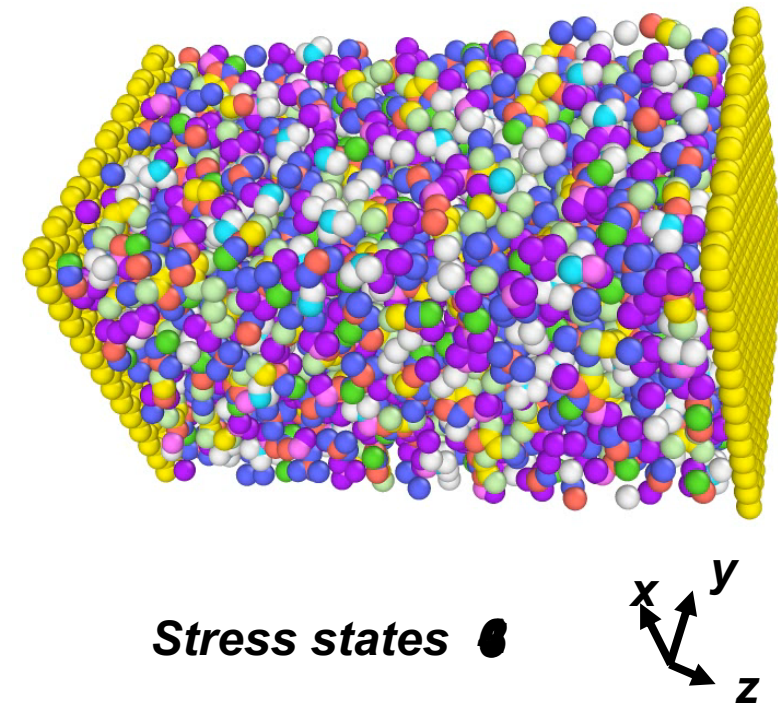


- PACKMOL, LAMMPS, OVITO, Constant potential method, OPLS AA forcefield
- *Equilibration*: 15 ns at 25°C in the NVT ensemble
- *Dynamic run*: Engineering strain rate = 0.001/*f*s

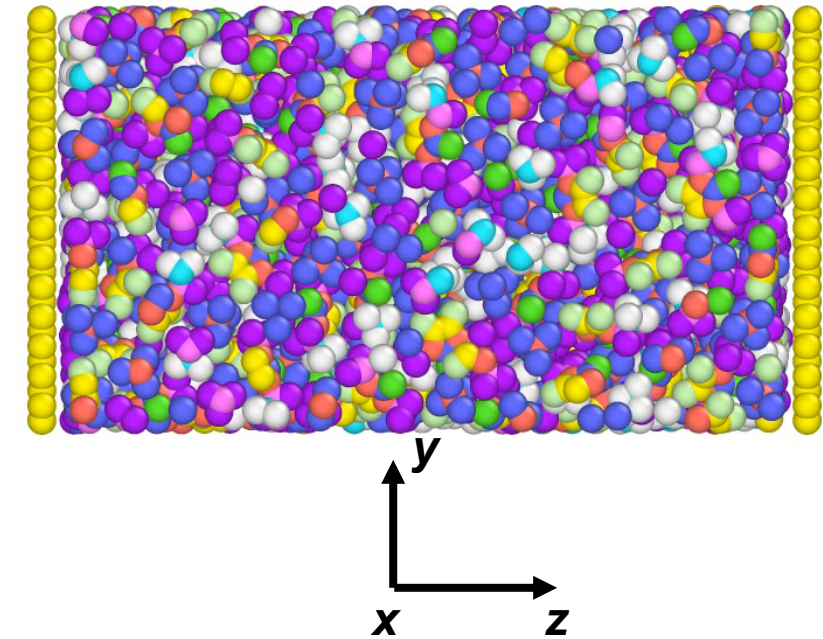
Roy et al. (under review)

# Compression and Stretching

## Compression of SC



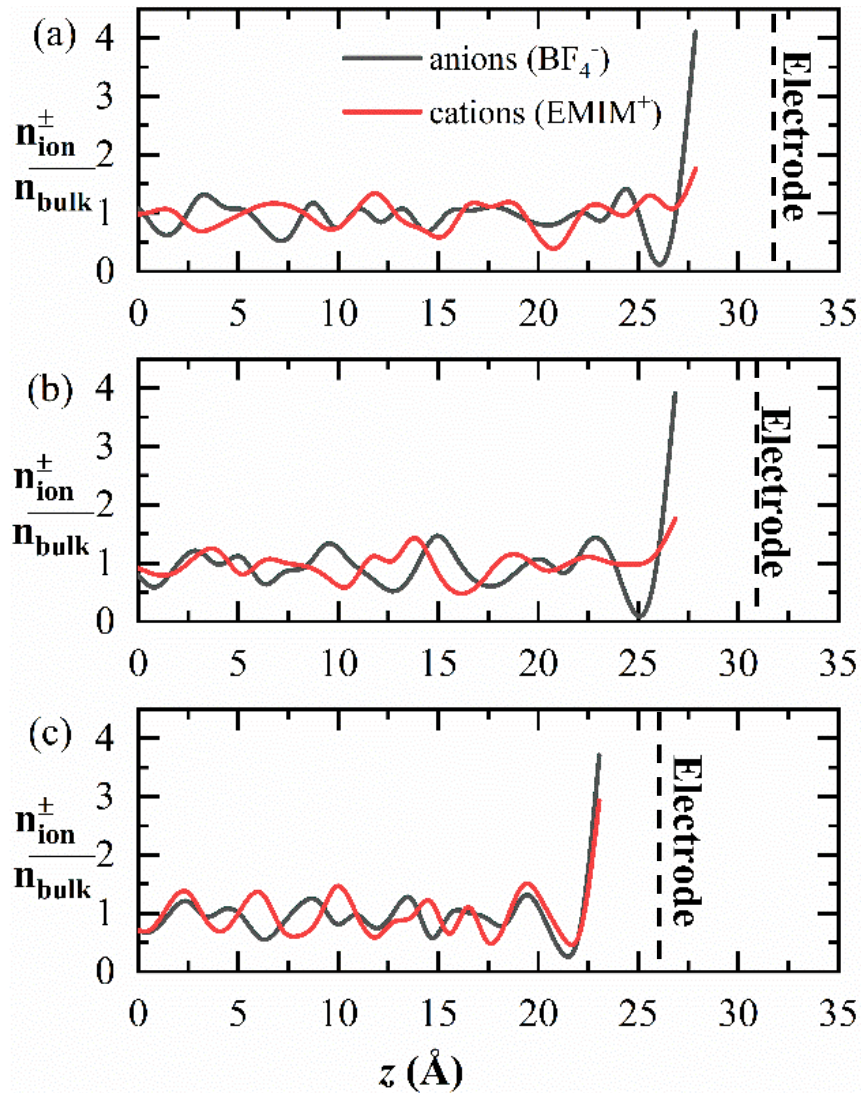
## Stretching of SC



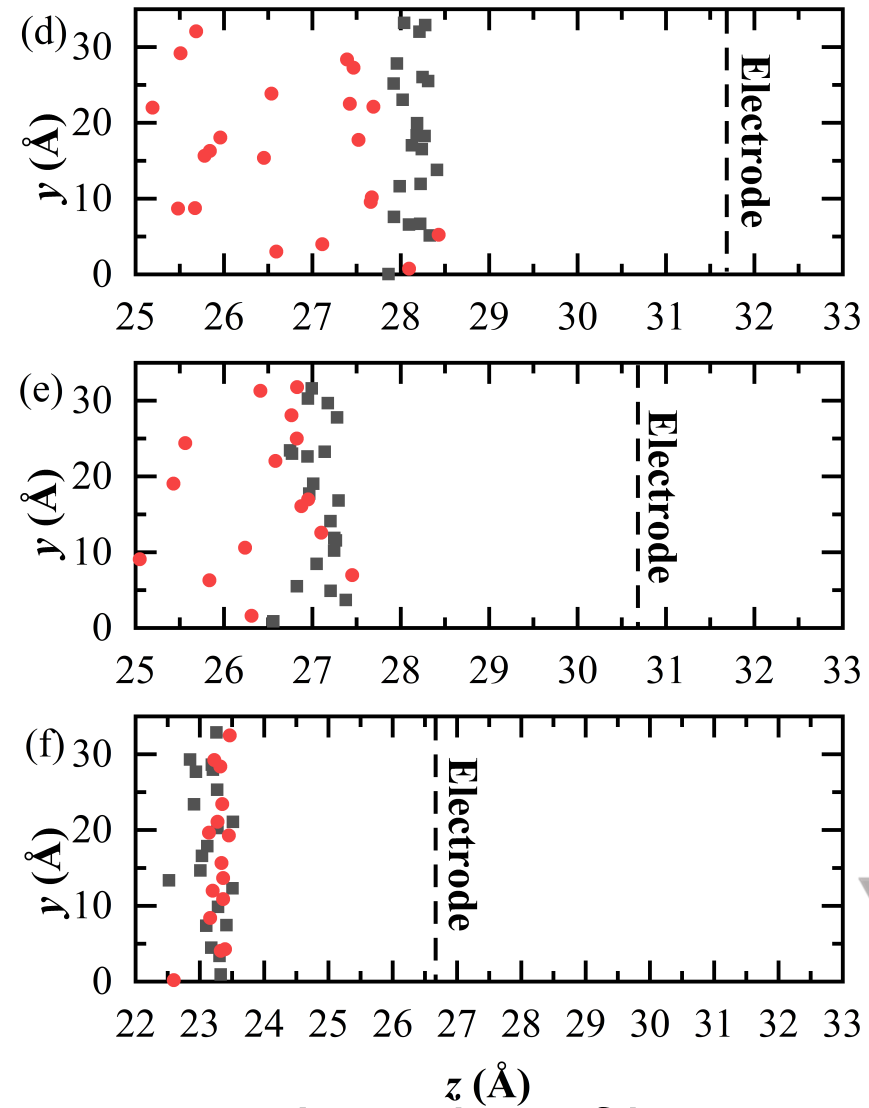
- **Compression/Stretching** was achieved keeping all parameters in equilibrium
- A potential difference of **4V** was used for all simulations



# Behaviour of electrolyte

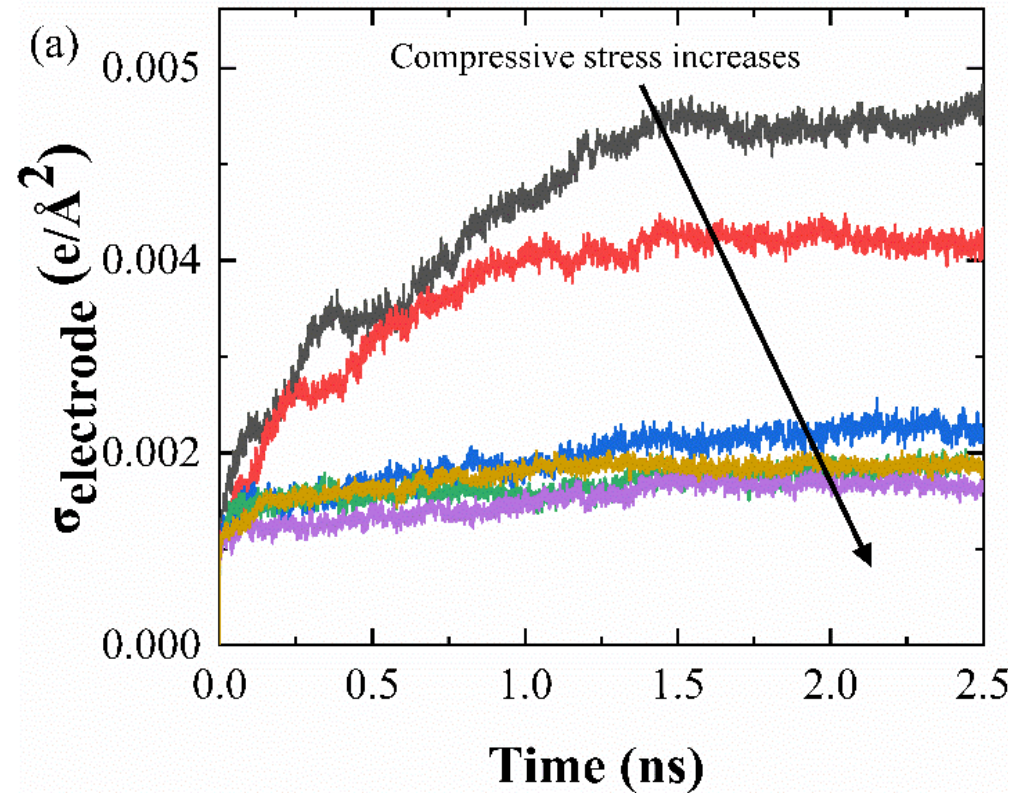


*Normalised charge density*

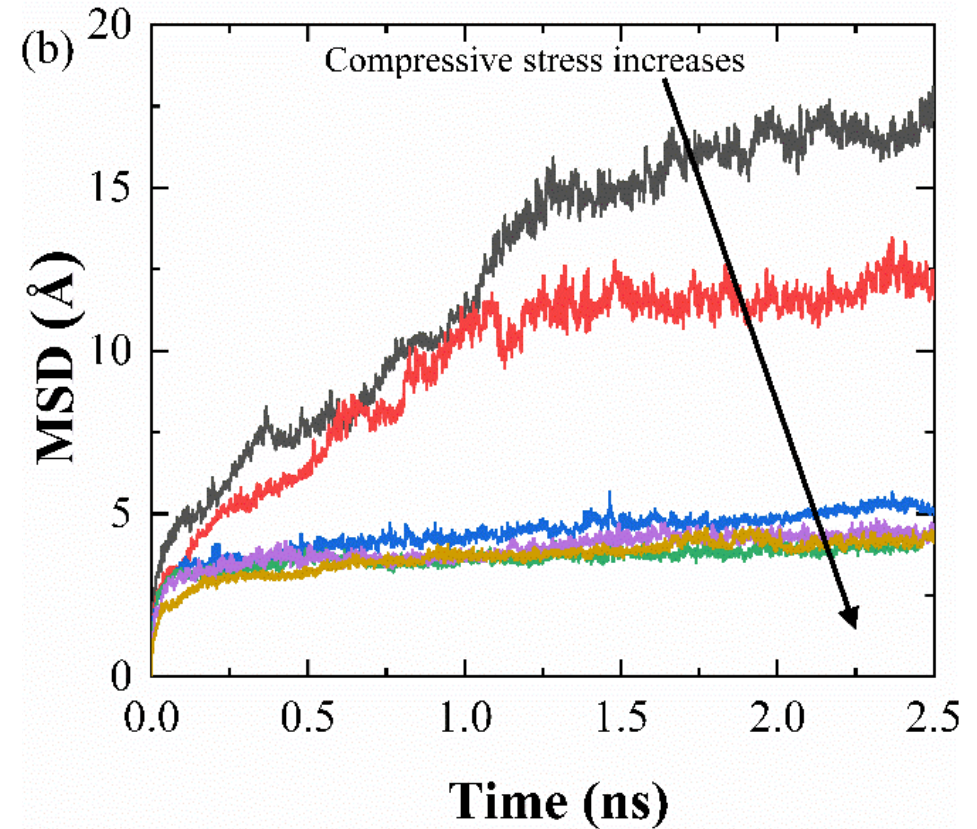


*Location of ions*

# Behaviour of electrode



*Charging dynamics*

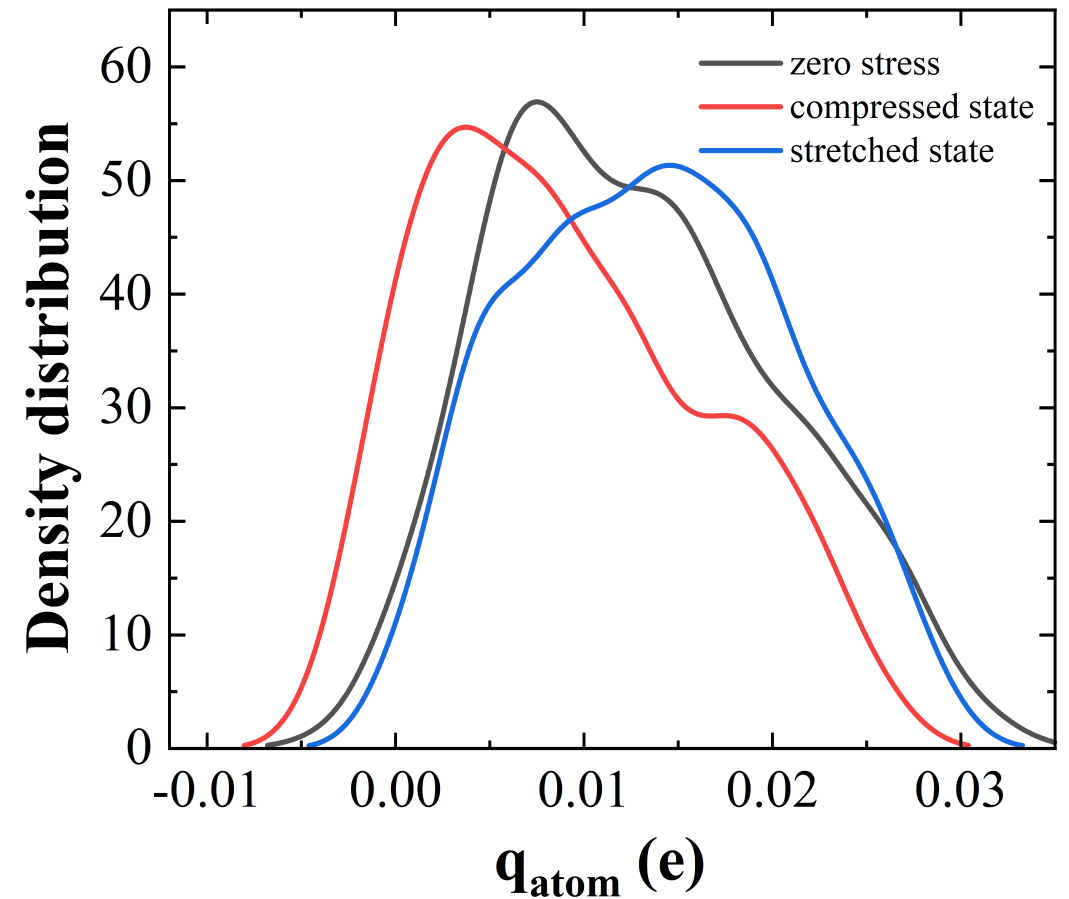
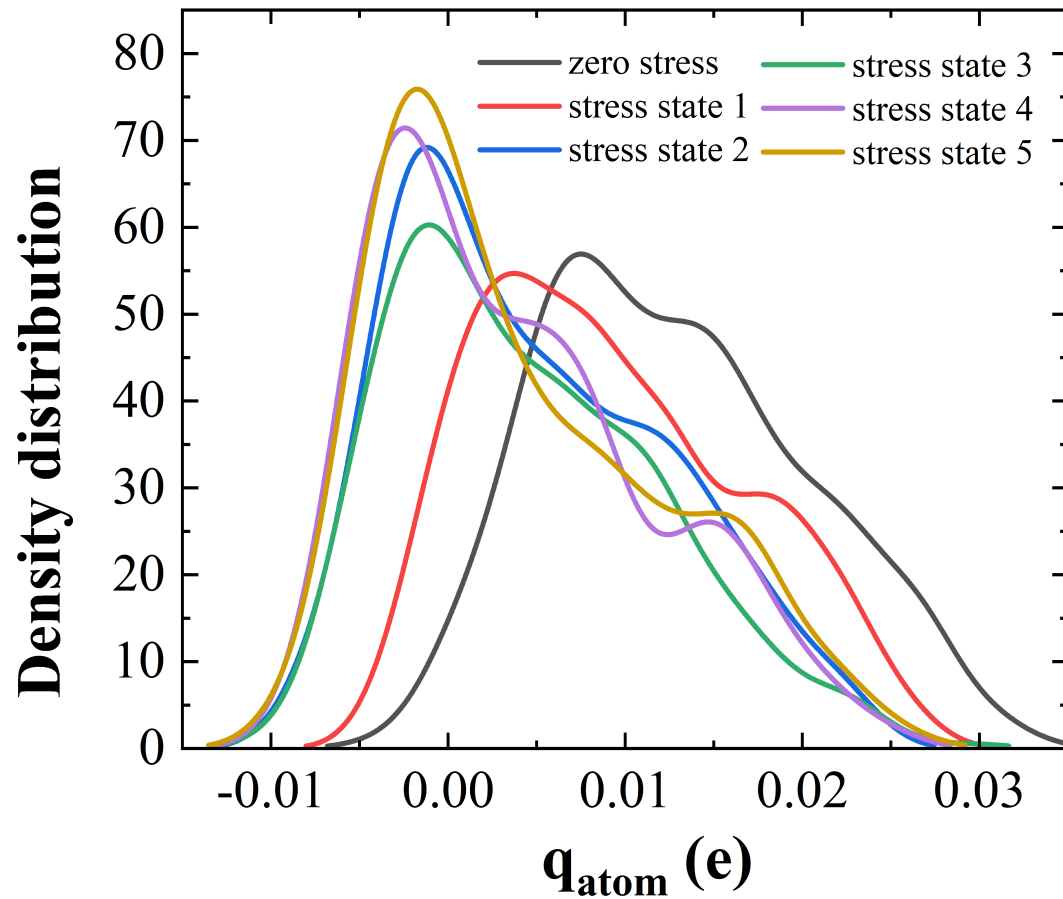


*Mean square displacement*

- MSD of ions is directly proportional to the **reduction in electrode charge density**
- Increasing compression leads to **low charge storage**

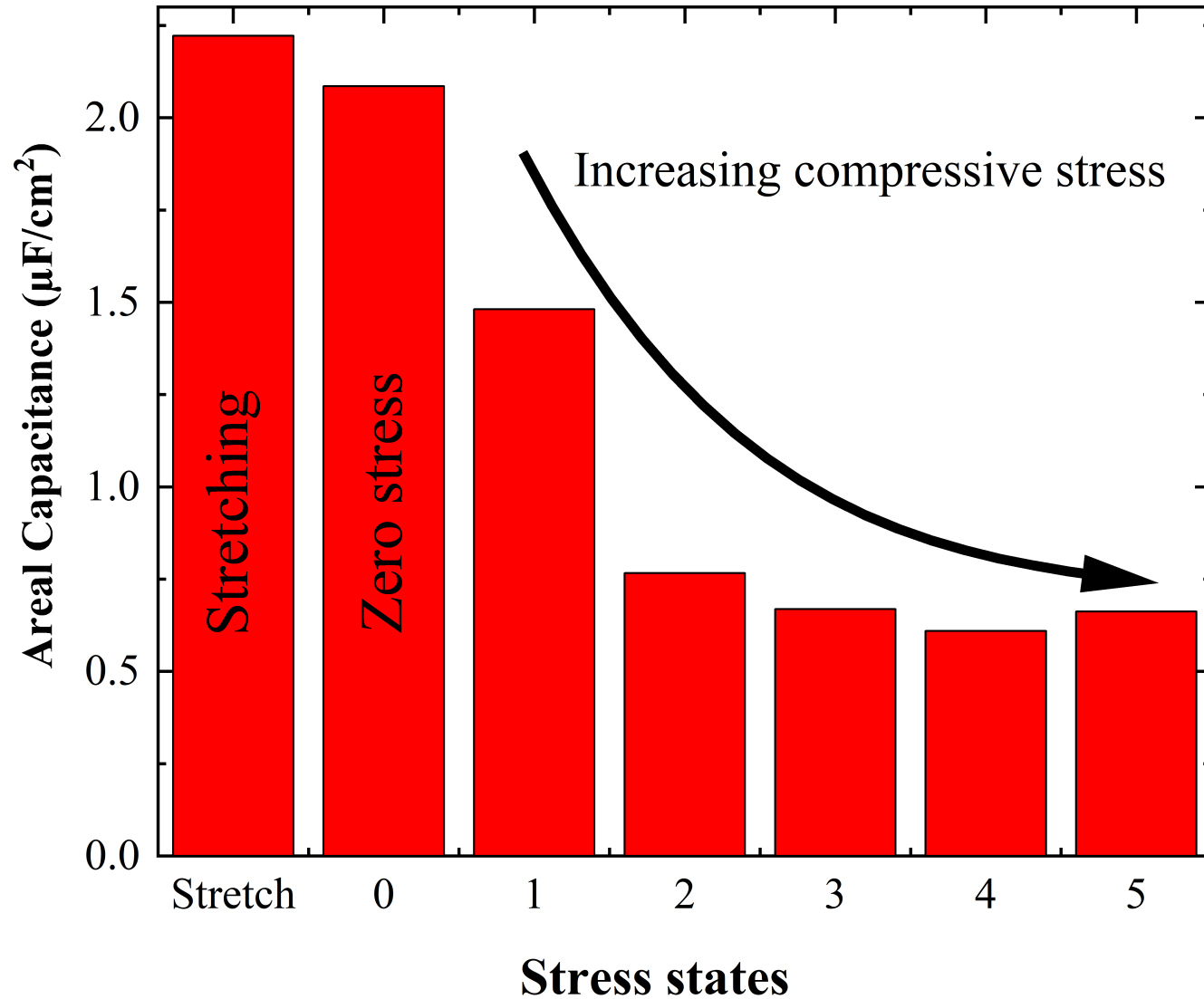


# Behaviour of electrode



*Density distribution of electrode atom charge*

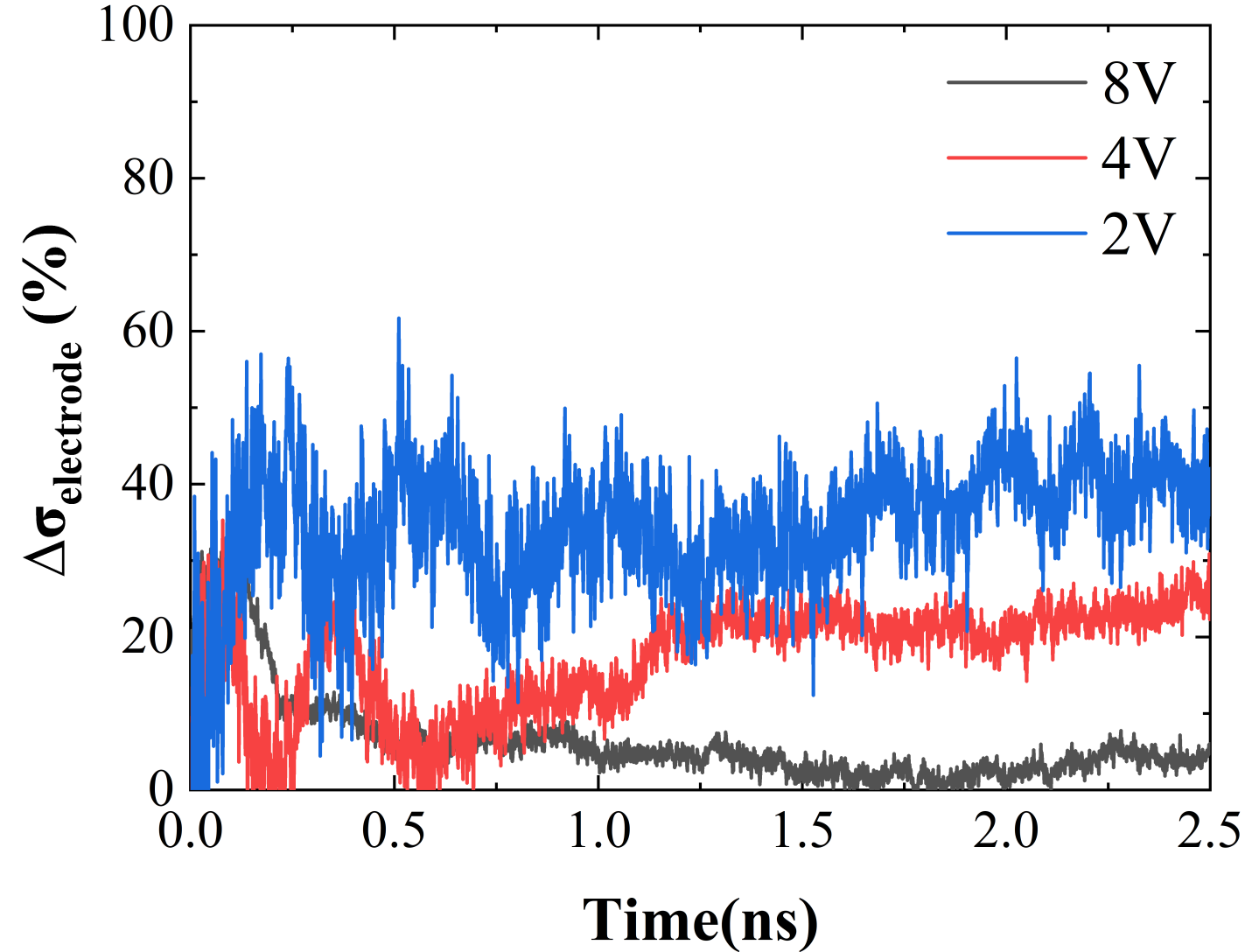
# Double layer capacitance



- **Tension-compression asymmetry**
- **Capacitance reduces** with compression



# Compression at different voltages



- Charge density **fluctuations minimise** with increase in potential
- Capacity retention at **higher potentials**

- **Strain induced electrochemical behaviour** of IL based SC using molecular dynamics simulations
- **Low compression** showed a **reduced performance** in terms of charge density in the electrodes (29%) while **stretching improved performance** (7%)
- **Higher potential** leads to better **capacity retention with compression**



# Acknowledgment



***Thank you***

<https://www.imperial.ac.uk/people/t.roy>

<https://www.imperial.ac.uk/electrochem-sci-eng>