Molecular dynamics simulations of a supercapacitor with ionic liquid electrolytes

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Supercapacitors (SCs) / Ionic liquids (ILs)

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

• 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
Compression and Stretching

Compression of SC

- Compression/Stretching was achieved keeping all parameters in equilibrium.

- A potential difference of 4V was used for all simulations.

Stretching of SC
Behaviour of electrolyte

Normalised charge density

Location of ions

Increasing compressive stress
Behaviour of electrode

Charging dynamics

- MSD of ions is directly proportional to the reduction in electrode charge density

- Increasing compression leads to low charge storage

Mean square displacement
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

\[ \Delta \sigma_{\text{electrode}}(\%)
\]

Time(ns)

- Graph showing compression at different voltages
- Lines for 8V, 4V, and 2V potentials
- Y-axis represents change in conductivity (\(\Delta \sigma\)) expressed as a percentage
- X-axis represents time in nanoseconds (ns)

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Conclusion

• **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**
Thank you

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