ENHANCING MEAN-FIELD MODELS FOR ELECTRIC DOUBLE LAYER CAPACITORS

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Applications
- Stabilizing the national power grid
- Efficient, eco-friendly energy stores
  - Buses and cars

Limitations
- Energy does not last long
- Too expensive for widespread use
ELECTRIC DOUBLE LAYER THEORY
Acknowledging limitations of Gouy-Chapman theory

Improving theoretical models with computer simulations

Making supercapacitors more efficient

Reducing costs and promoting sustainability

DESIGN AND IMPACT OF RESEARCH
1. Write LAMMPS script for EDL simulation

2. Setup script for various configurations
   - Change relative and absolute ion sizes

3. Run script on CNSI/LANL supercomputers
   - Enables several simulations to run at once
   - Simulations take just over 1 day to run
ADVANCING THE MODEL

4. Graph charge concentrations vs. distance from electrode to show real results

5. Use MD data to guide development of theory
MOLECULAR DYNAMICS DEMO
EFFECTS OF DIFFERENT ION SIZES

Density profile of attracted ions

Charge Concentration

Distance

Increasing charge on electrode
EFFECTS OF DIFFERENT ION SIZES

Density profile of repelled ions

Charge Concentration vs Distance

Increasing charge on electrode
EFFECTS OF DIFFERENT ION SIZES

Profile of net charge

Increasing charge on electrode
EFFECTS OF LARGE ION SIZES

Density profile of attracted ions

Charge Concentration

Distance

Increasing charge on electrode
EFFECTS OF LARGE ION SIZES

Density profile of repelled ions

Charge Concentration vs Distance

Increasing charge on electrode
Predicted oscillations did occur
- Key is volume fraction, though, not just relative ion sizes

Found regime where Gouy-Chapman theory fails
- Does very good job, though, for certain setups

Combine relative and absolute ion size changes
Develop mathematical model of our results
Translate our developments to industry
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VOLTAGE PROFILE (OSCILLATING CASE)