Asian Deans' Forum 2026

THE RISING STARS

Women in Engineering Workshop

SEP 13 – 15 | HKUST, Hong Kong

COMPUTATIONAL MATERIALS DESIGN · POSTER

Bridging Molecular Simulation and Data-driven Modeling for Electrolyte Design in Lithium Metal Batteries

Minhee Park | PhD Graduate, Seoul National University · Theoretical and Computational Soft Matters Lab

THE PROBLEM

The next leap in energy density depends on a liquid nobody can look inside.

Lithium metal is the highest-capacity anode known: **3860 mAh g^{-1}**, ten times graphite, at **-3.04 V** vs. SHE. It stays out of products because the electrolyte beside it decomposes: dendrites grow and efficiency collapses.

What decides the outcome (coordination, transport, oxidation) is molecular and out of experimental reach; solvent × salt × additive is a space trial and error cannot cover.

3
Scales joined in one workflow: quantum, atomistic, statistical

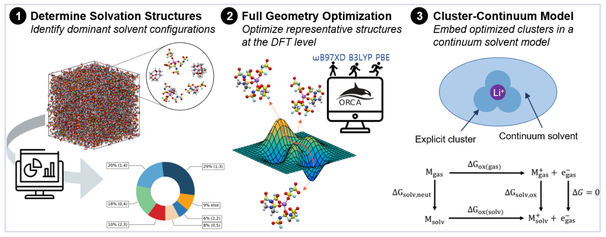
288
Electrolyte systems simulated, plus 308 database solvents

0.79
Cross-validated R^2 for Coulombic efficiency, from structure alone

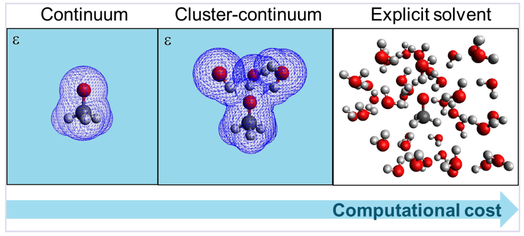
2-6
Components per formulation the model takes without retraining

METHODOLOGY

One pipeline, three resolutions: MD · DFT · machine learning, applied together throughout



The stability window is computed from the speciation the liquid actually holds, not from one representative molecule.



Quantum treatment where coordination happens, continuum elsewhere: explicit-solvent accuracy at a fraction of the cost.

01 · SIMULATE & 02 · QUANTIFY

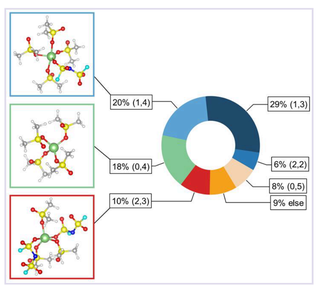
APPLE&P polarizable MD with induced dipoles on every atom, NPT at 333 K, 40.5 ns, where fixed-charge fields hold charges constant and run 10–100× too slow. The first solvation shell is then treated explicitly at the quantum level and the bulk implicitly: geometries at PBE and B3LYP, 6-31+G(d,p), single-point ωB97X-D3 with CPCM, giving explicit-solvent accuracy at a fraction of the cost.

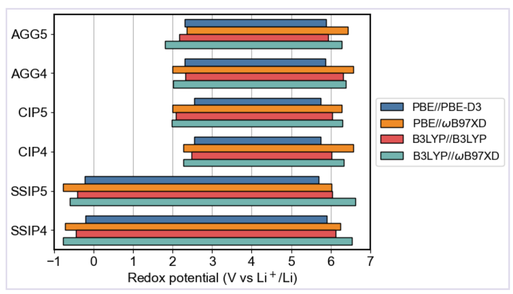
03 · PREDICT

Each component enters as its own molecular graph from SMILES; four GATv2 layers with four attention heads, mean pooling scaled by molar concentration, three-layer MLP head. Pre-trained on 500 molecular dipole moments.

PART 1 · FOUNDATION

A stability framework you can trust: the window is a population, not a molecule





No single complex represents the electrolyte: contact pairs lead at 29% and 5-coordinate species cannot be left out, and only hybrid functionals reproduce the ensemble's window.

① A generalizable ESW framework

MD speciation weighted into cluster-continuum DFT. Benchmarked on EMC + $LiPF_6$, where contact-pair oxidation at 6.36 V matches experiment, and within 1% of full ωB97X-D3 at a fraction of the cost.

② Speciation → interphase chemistry

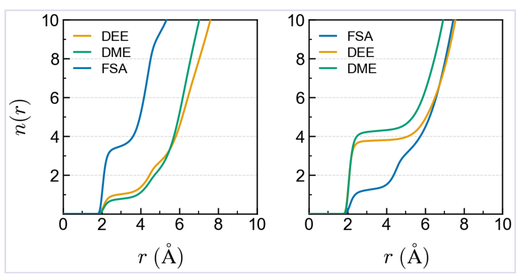
Ion pairs and aggregates reduce ~2 V above solvent-separated pairs, with the LUMO localised on the anion; S–F dissociation then sends fluorine to Li^+, the LiF-rich SEI precursor.

RAISED

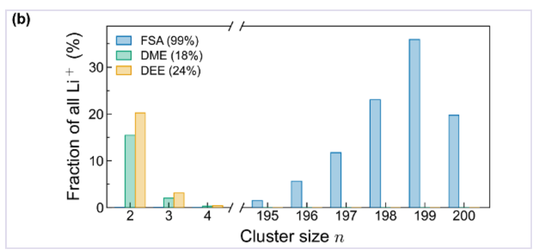
If speciation governs stability, does it also govern transport, in a real and unstudied electrolyte?

PART 2 · TEST

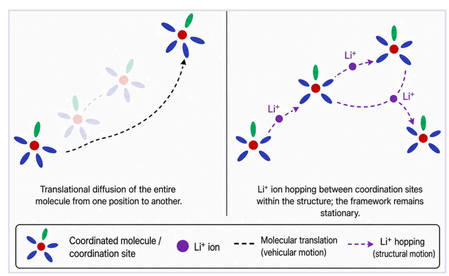
A weakly solvating electrolyte, structure to interphase: FSA (ε = 52.46) against DME (7.2) and DEE (3.8)



In FSA lithium is coordinated by its anion rather than its solvent, the reverse of the ethers.



FSA is not a solution of discrete ions but one connected network.



Weak solvation changes the transport mechanism, not merely its rate.

③ Speciation sets the transport mechanism

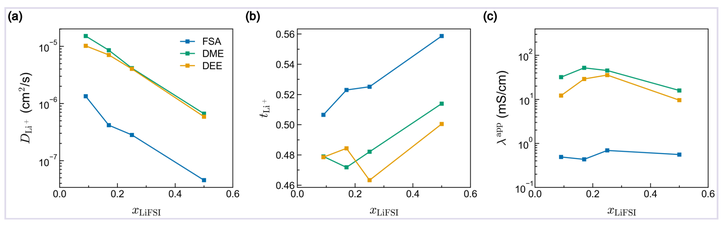
Residence times are one to three orders shorter in FSA, which is why low conductivity and diffusivity coexist with a transference number above 0.5. Van Hove correlations, Green–Kubo currents and a Haven ratio α ≈ 0.15 agree.

④ Ensemble-invariant redox stability

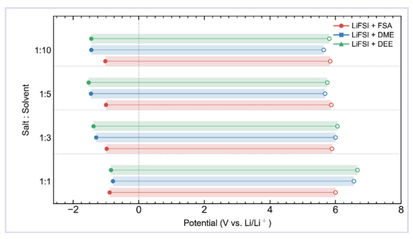
Solvation collapses the LUMO gap by 97%, so FSA's window is composition-insensitive and anion reduction wins regardless of coordination, verified at the interface by cryo-TEM and EELS.

RAISED

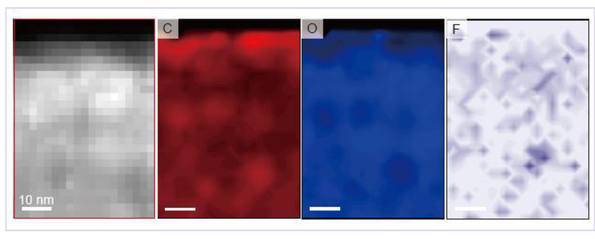
Can these structural principles scale to thousands of candidates without running MD and DFT for each one?



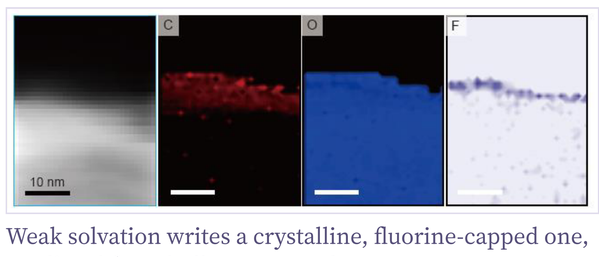
Conductivity and transference number pull against each other; weak solvation buys the second at the cost of the first.



Once solvation is weak, concentration stops being a design knob.



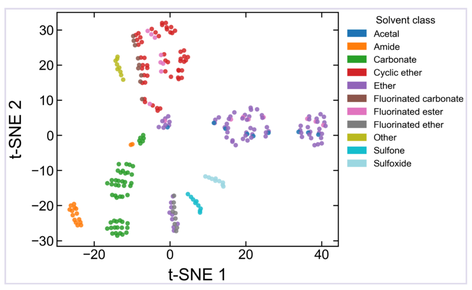
Strong solvation writes an organic, amorphous interphase.



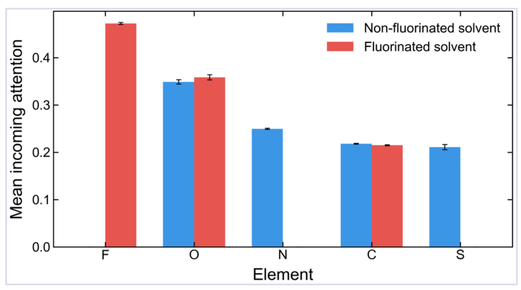
Weak solvation writes a crystalline, fluorine-capped one, predicted from bulk structure alone.

PART 3 · SCALE

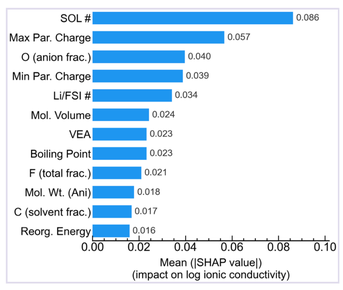
Learned screening over whole formulations, and the model rediscovers the chemistry



The model organises electrolytes by a chemistry nobody encoded for it.



It learns to look where the physics says to look.



Composition weighs as heavily as molecular identity.

⑤ An architecture that reads mixtures

Trained on 288 MD systems, 308 database solvents and 147 measured formulations. Graph learning beats fixed descriptors on conductivity (R^2 0.528 → 0.615) and reaches $R^2 = 0.79$ on Coulombic efficiency for two- to six-component formulations.

⑥ Chemistry recovered from the latent space

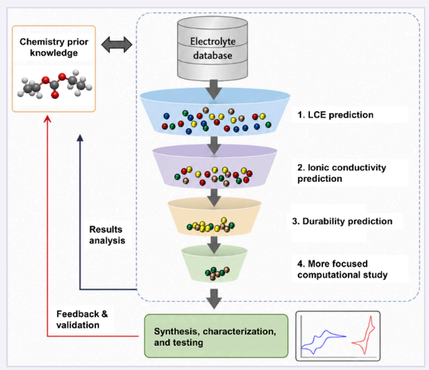
High-efficiency formulations cluster at high fluorine and low oxygen: the trade-off Parts 1–2 derived from physics, recovered from data.

CLOSES THE LOOP

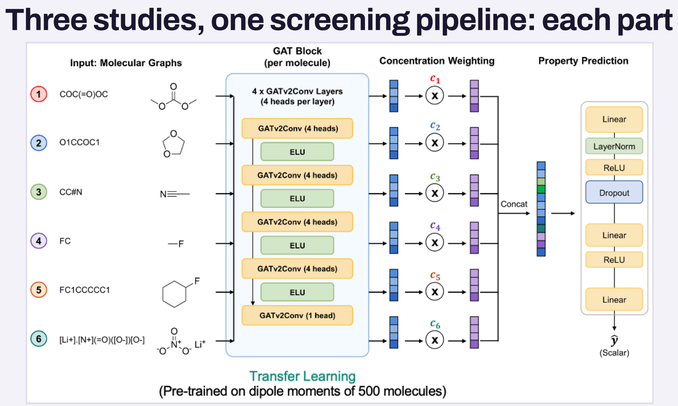
The learned model rediscovers the physics, so its predictions hold beyond the compositions ever simulated.

THE COMPLETE WORKFLOW

Three studies, one screening pipeline: each part answers the question the previous one raised



The three studies compose into one filter that runs before any experiment.



One graph per component is what makes a real mixture predictable at all.

Part 1 built a stability framework that trusts the whole solvation ensemble, raising whether speciation also governs transport. **Part 2** answered that in a real weakly solvating electrolyte, where the same aggregated structure sets both hopping transport and a fluorine-rich interphase, raising whether the principles scale without MD and DFT per candidate. **Part 3** answered with a model whose attention rediscovers that physics, so a database can be narrowed by learned predictors before any simulation runs. Discovery stops being a search and becomes a filter.

NEXT

Grand-canonical MD under applied voltage, to capture the electric double layer.

Inverse design with the trained network as discriminator; active learning to pick what to compute next.

VALIDATION

Benchmarked against EMC + $LiPF_6$; interphase confirmed by cryo-TEM and EELS with Prof. Jungwon Park's group.

RECORD

Three first-author papers: J. Phys. Chem. C (2023), Energy Storage Mater. (2024), Chem. Eng. J. (2025); two more in preparation.

Co-author in Advanced Materials, ACS Nano and Small. Industry research with Hyundai Motor Group–SNU (2022–24); stay at Imperial College London (2025).

Organizers

THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY

UNSW SYDNEY

SEOUL NATIONAL UNIVERSITY

NUS National University of Singapore

NTU

UTokyo

Tsinghua University