

Motivation

➤ Advancement in battery technology requires...

➤ Novel electrolyte materials that mitigate environmental hazards

➤ Multi-scale resolution of life-limiting mechanisms

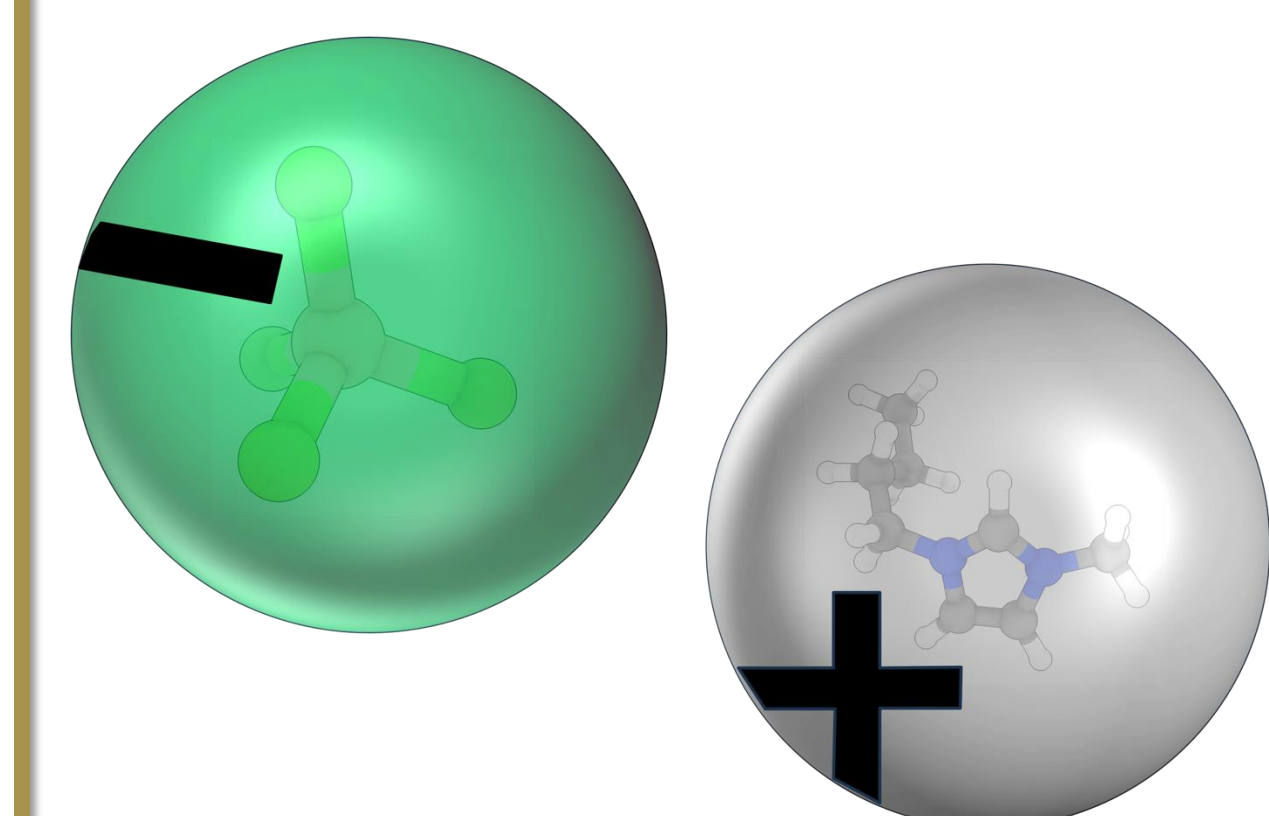
➤ Higher energy densities at electrochemical interfaces



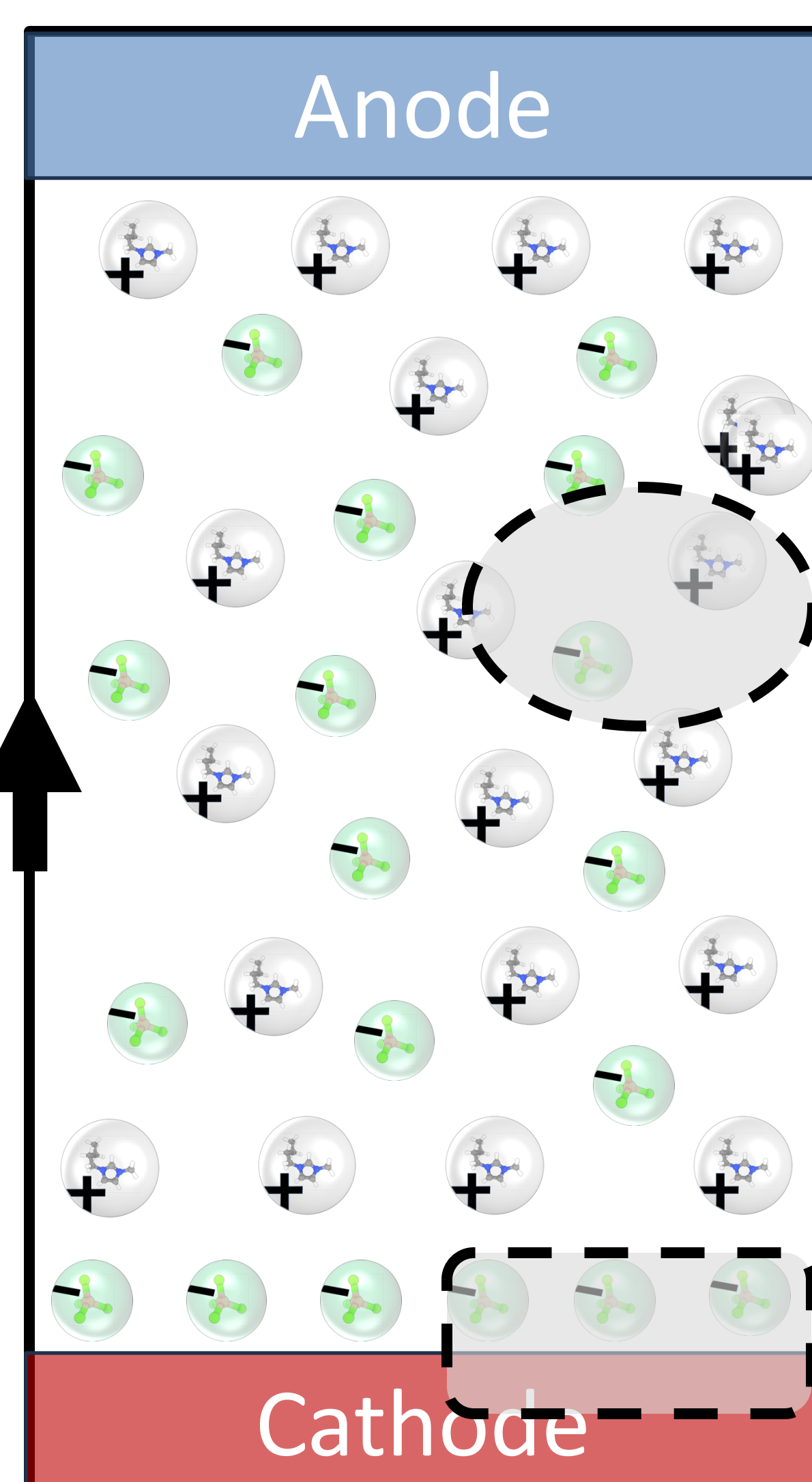
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Ionic Liquids are...

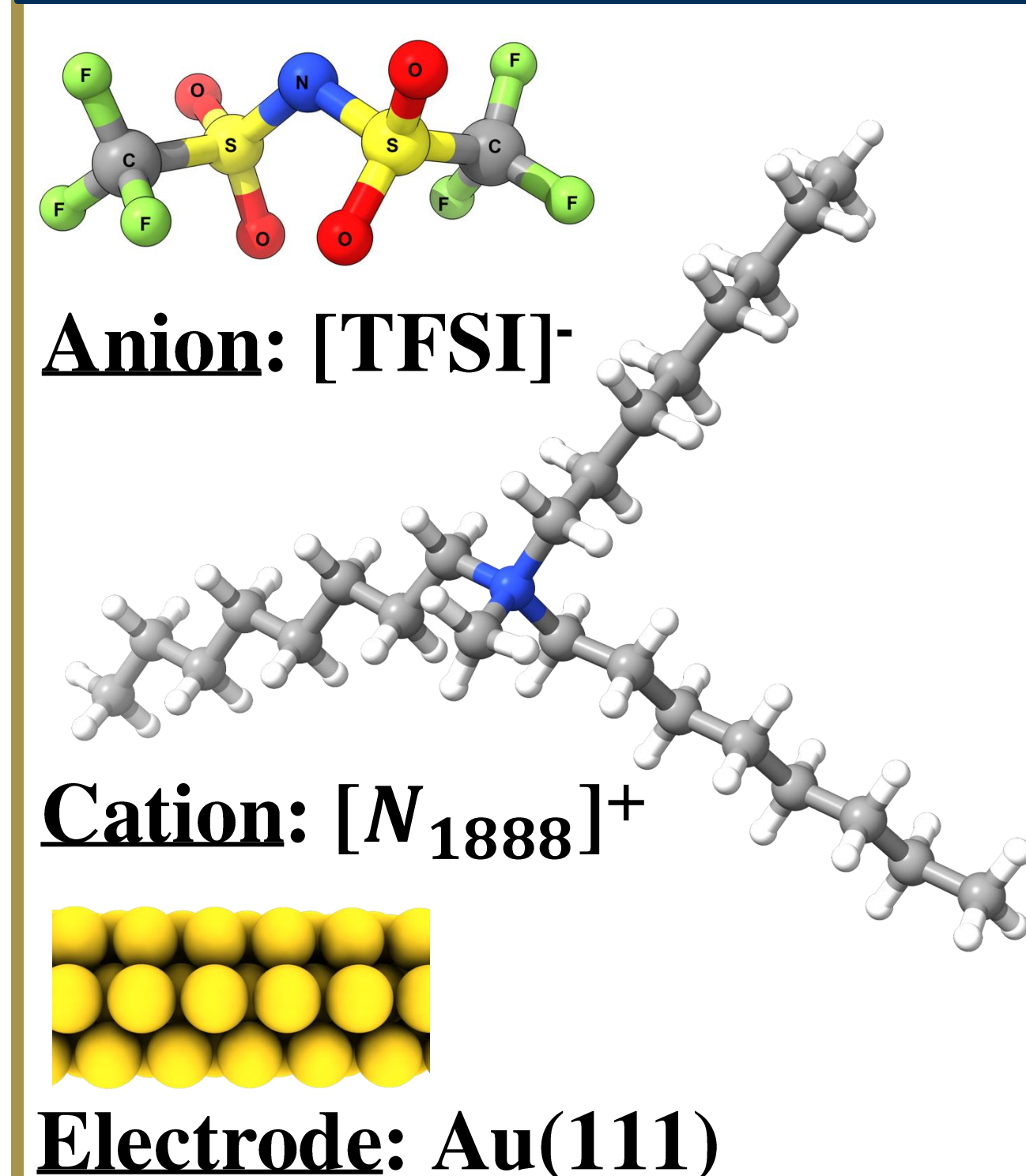
- Non-flammable
- Thermally stable
- Negligible vapor pressure
- Easy to handle



How can we study **model systems** to improve battery **lifetime and performance**?



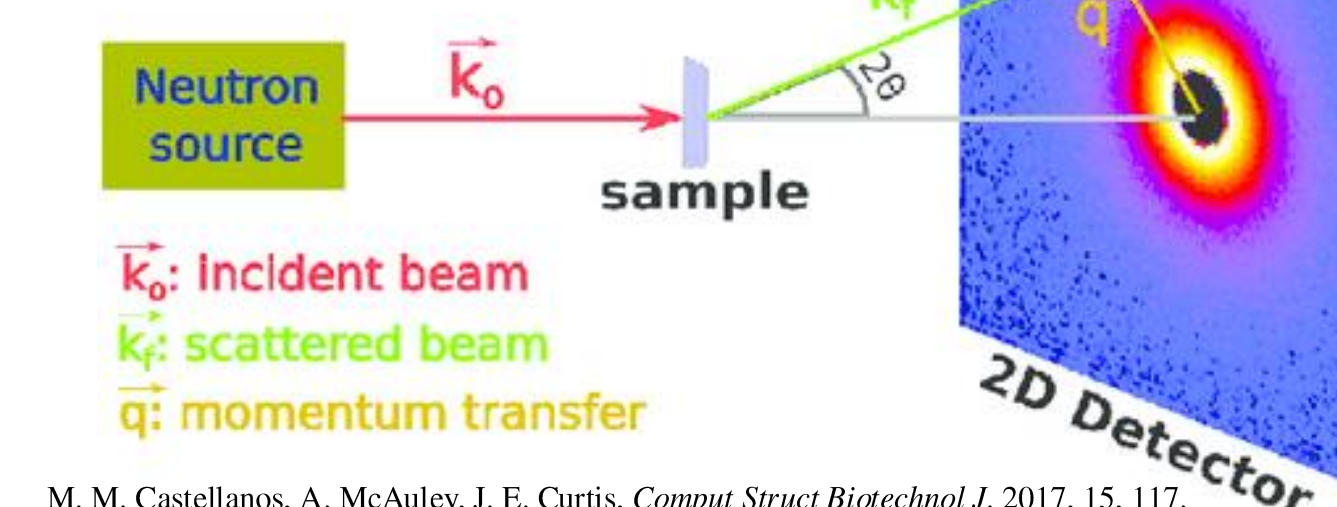
Methods



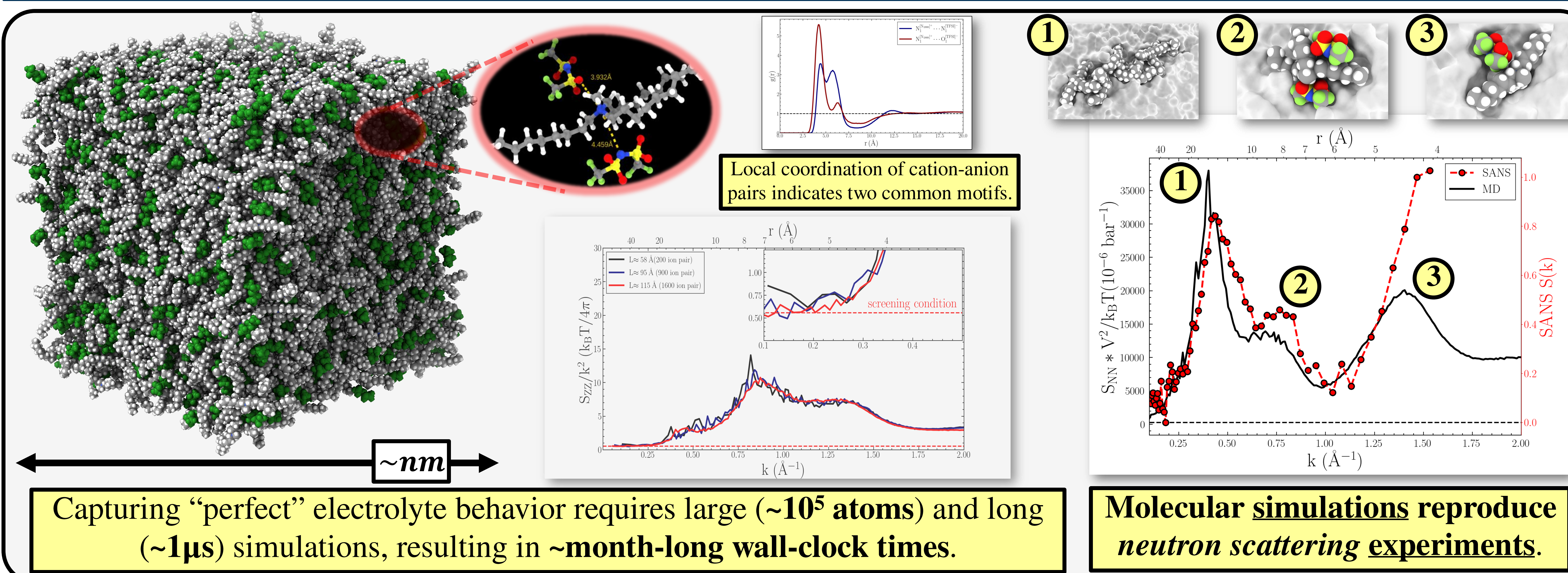
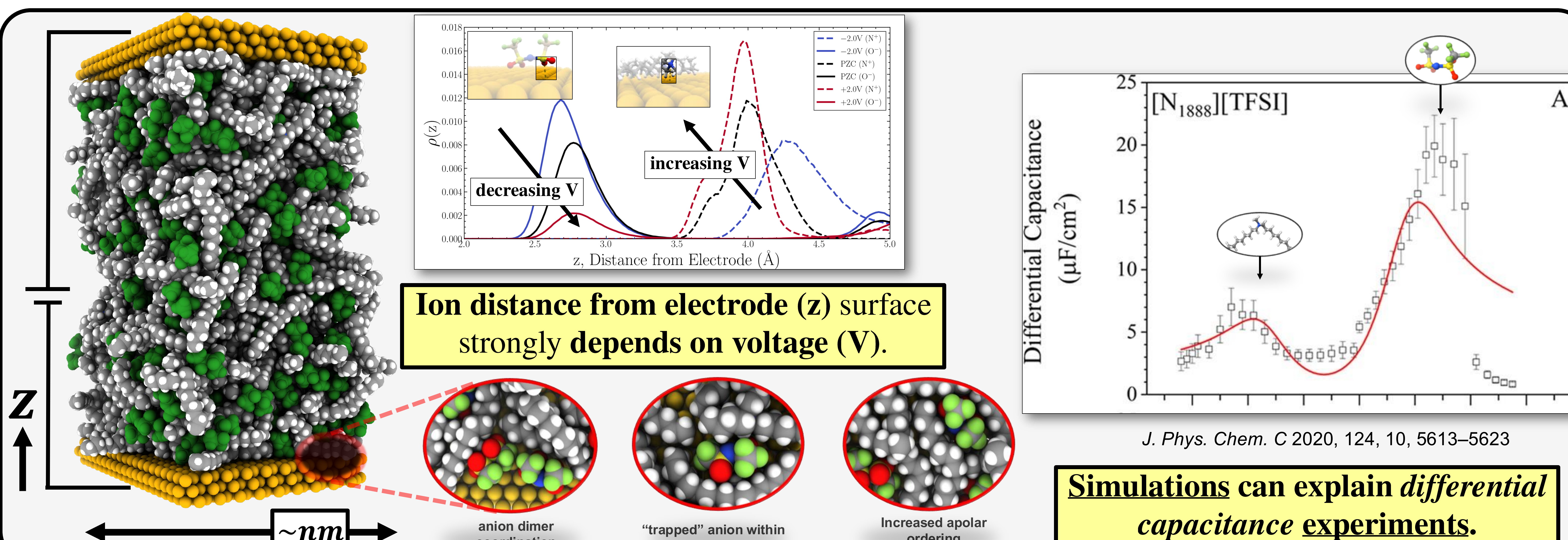
“First Principles” Simulations



Neutron Scattering Experiments



M. M. Castellanos, A. McAuley, J. E. Curtis, *Comput Struct Biotechnol J.* 2017, 15, 117.

Bulk-Phase Electrolyte Structure: [N₁₈₈₈][TFSI]Electrode-Electrolyte Interface: Au(111) | [N₁₈₈₈][TFSI]

Conclusions and Future Work

- Paired with **experiments**, atomistic **simulations** provide insight on **bulk-phase** and **interfacial behavior** of an ionic liquid/electrode system.
- Model systems

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