TARTU ÜLIKOOL
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MD simulations of ionic liquids

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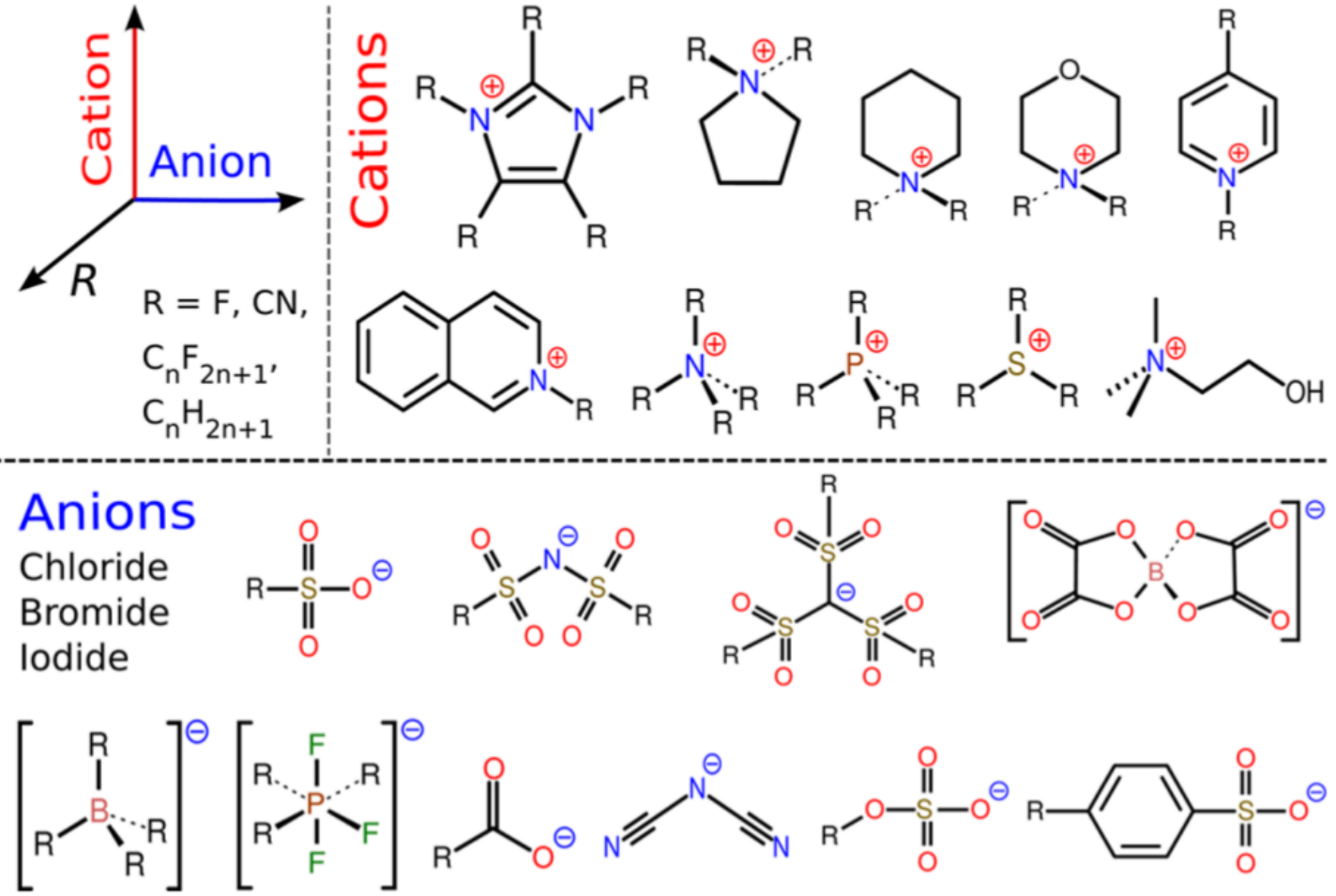
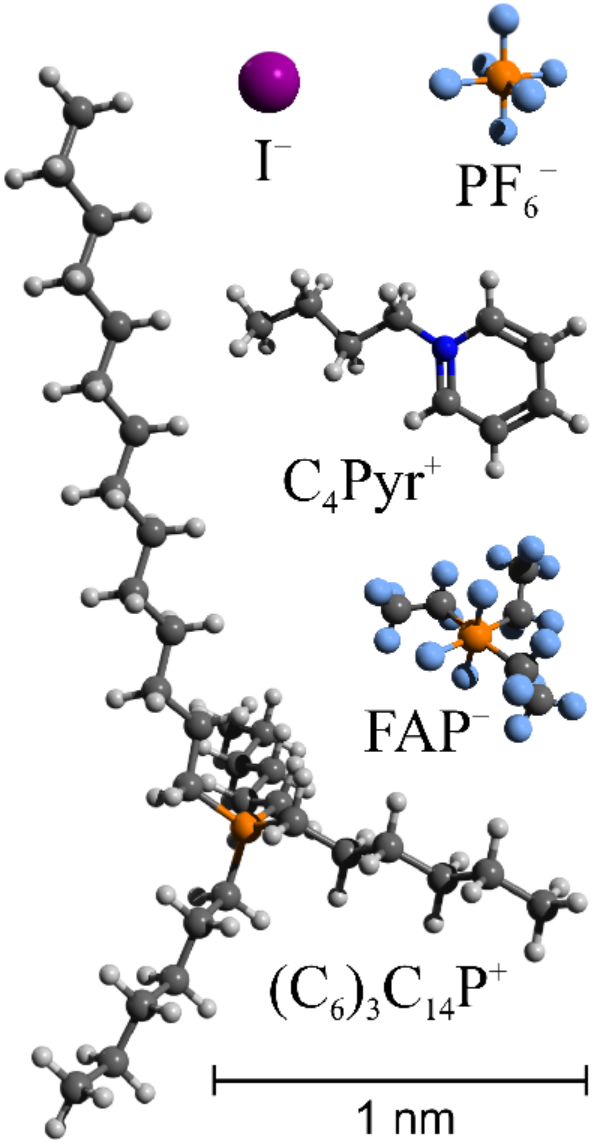
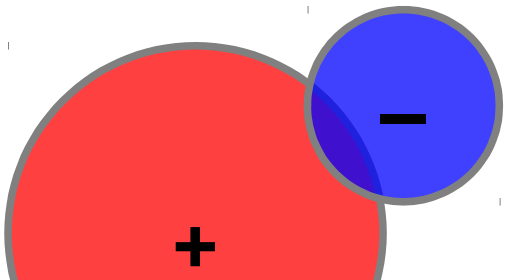
Ionic liquids models





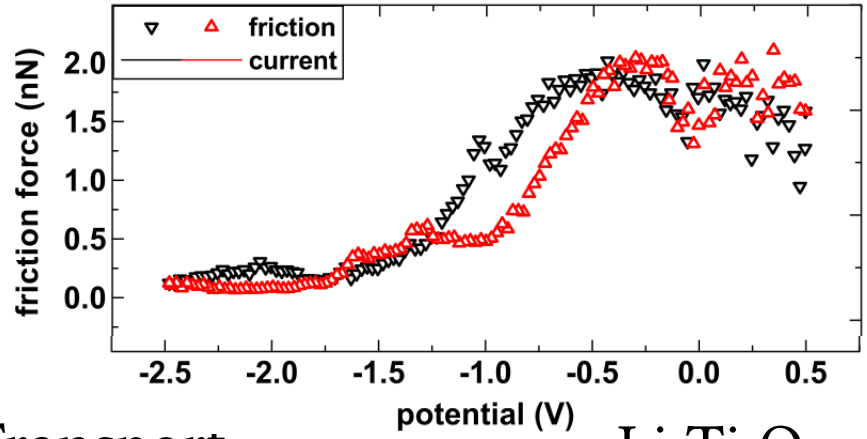
Coarse grained model →



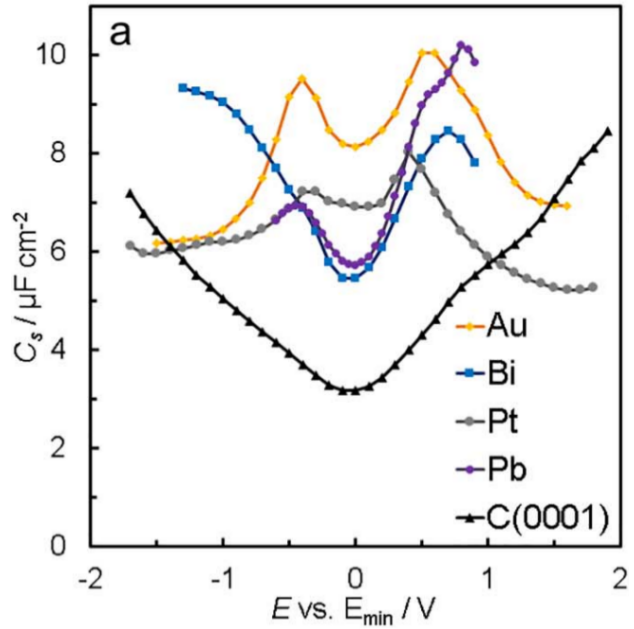
Experiment

1. J. Sweeney *et al.*, PRL 109 (2012) 155502–5.
2. O. Oll, T. Romann, C. Siimenson, E. Lust, *Electrochem. Commun.* 82 (2017) 39–42.
3. Y. Ishihara, K. Miyazaki, T. Fukutsuka, T. Abe, *J. Electrochem. Soc.* 161 (2014) A1939–A1942.

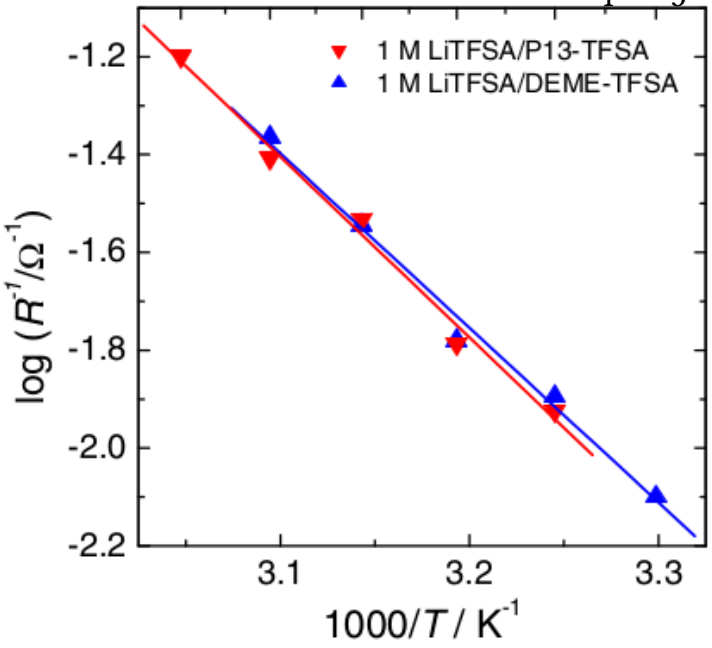
Friction Au(111)–BMPyrFEP



Capacitance Me–EMImBF$_4$



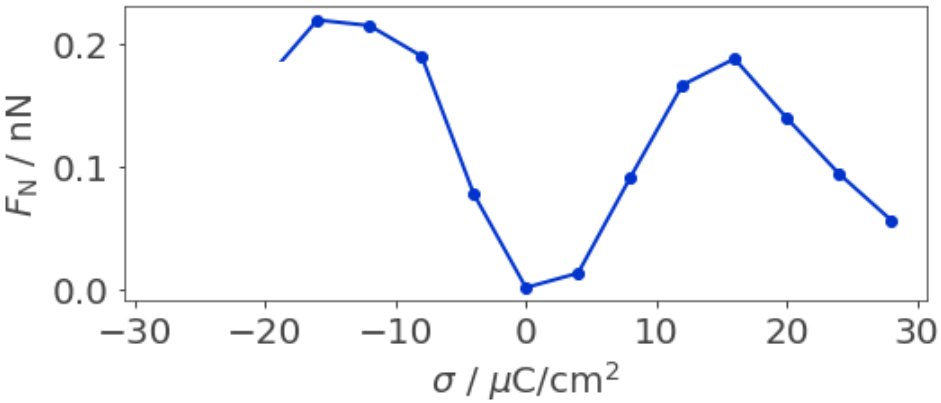
Transport $Li_4Ti_5O_{12}$



Calculations

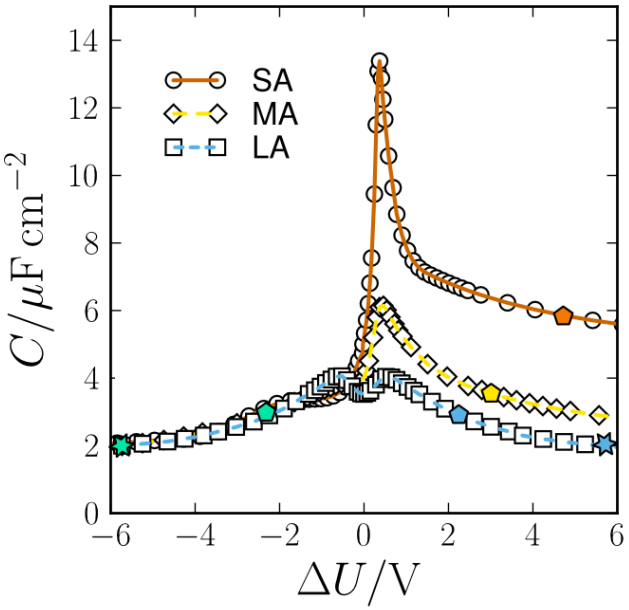
1. V. Ivaništšev, R. Capozza, in preparation
2. V. Ivaništšev, K. Kirchner, T. Kirchner, M.V. Fedorov, JPCM 27 (2015) 102101.
3. V. Ivaništšev, T. Mendez-Morales, R.M. Lynden-Bell, O. Cabeza, L.J. Gallego, L.M. Varela, M.V. Fedorov, PCCP 18 (2016) 1302

Friction



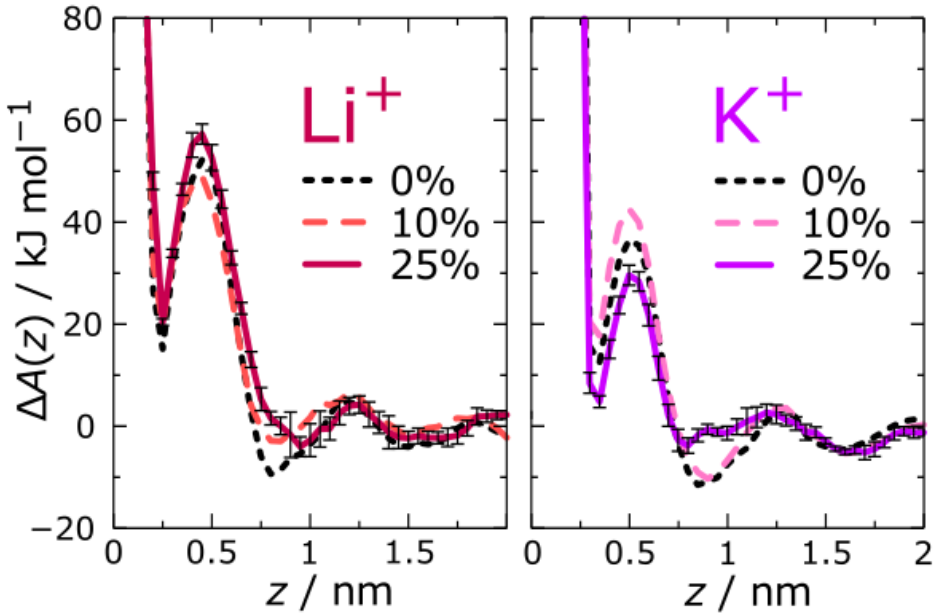
Capacitance

$$C \simeq aC_H U_\kappa^{a-1}$$

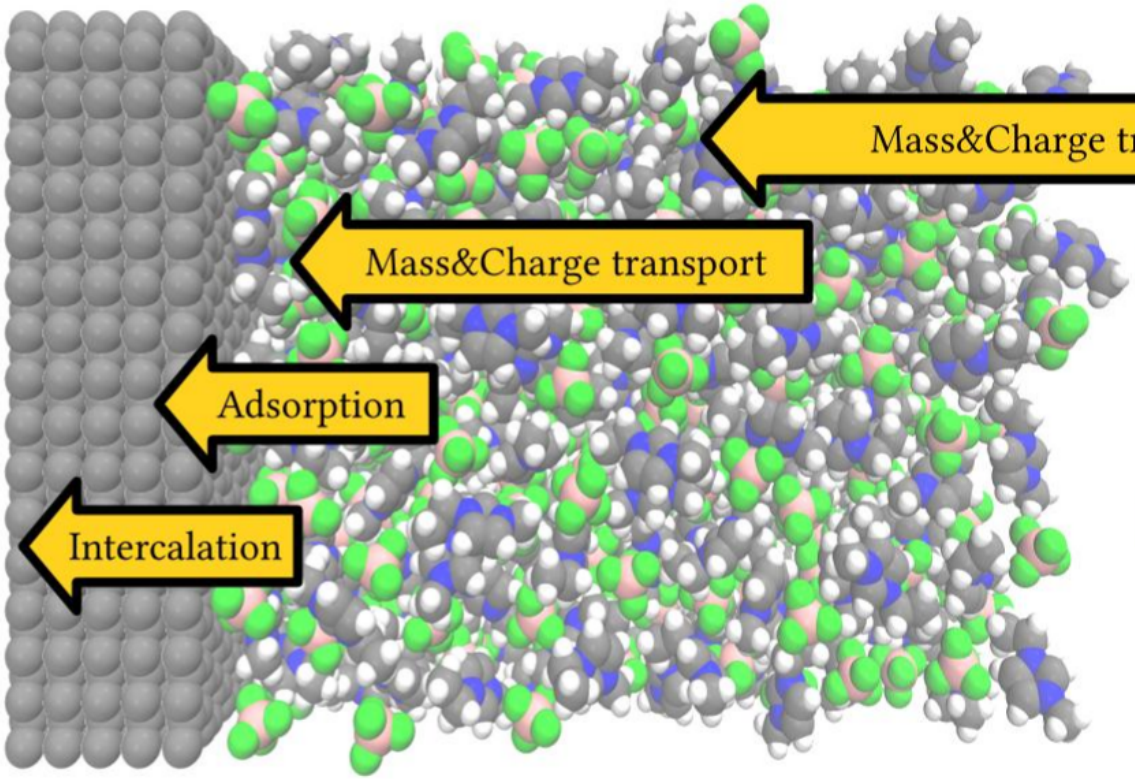


Resistance

$$R \propto \rho \exp[E_A/(k_B T)]$$



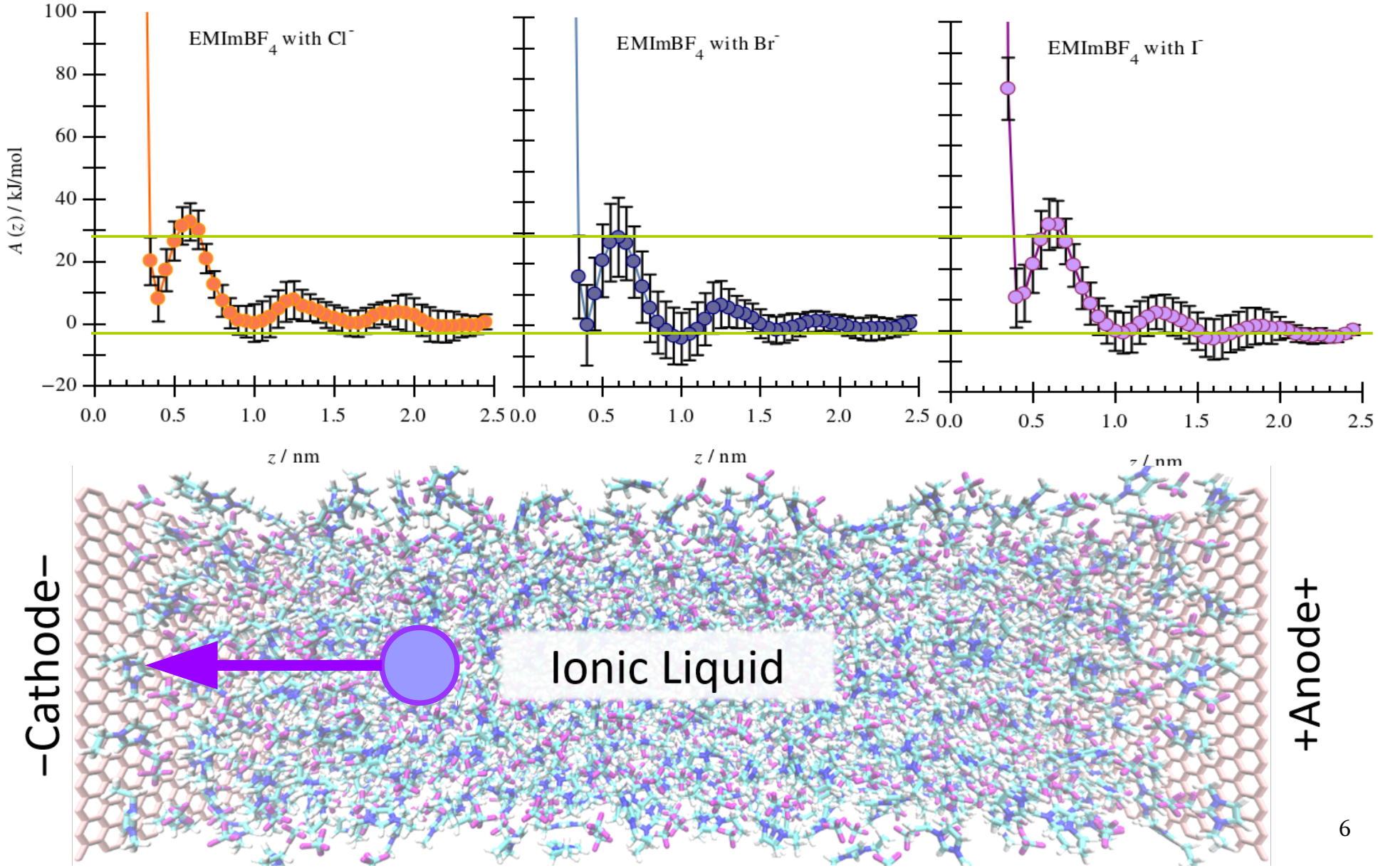
Dynamics at the interface



Computational screening:
(1) 2185 Li intercalation and 18226 Li conversion electrodes
build-a-battery.meteor.com
(2) 11000 electrolytes
M. Korth, PCCP 16 (2014).
(3) Few studies of interfaces

Figure 2. Ionic Liquid–Electrode Interface is an object of intensive research related to the development of novel types of Li-ion batteries and supercapacitors. Several pilot high-throughput studies have been performed recently to screen for electrodes and electrolytes, but there were no investigations of the interface, except for several case studies. The PI has been involved is some of the case studies and indicate that a pioneering high-throughput study can be made.

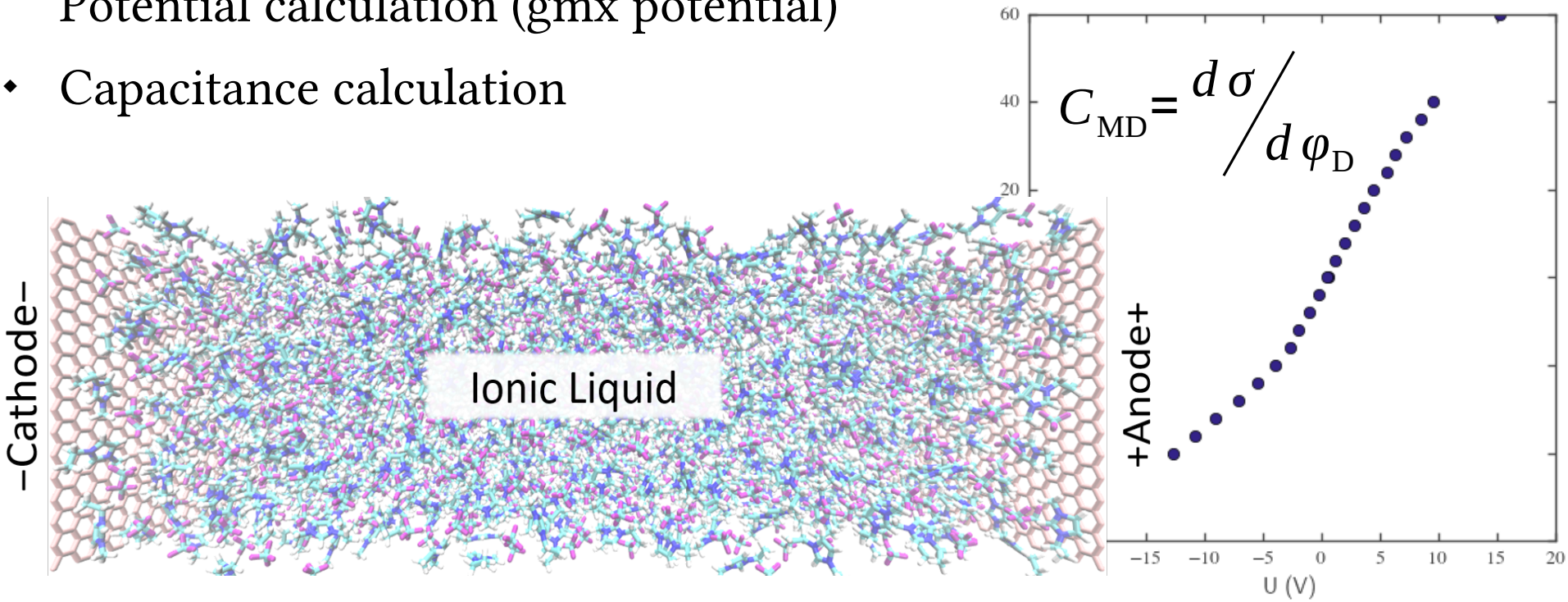
MD simulations & Potential of Mean Force



MD & capacitance

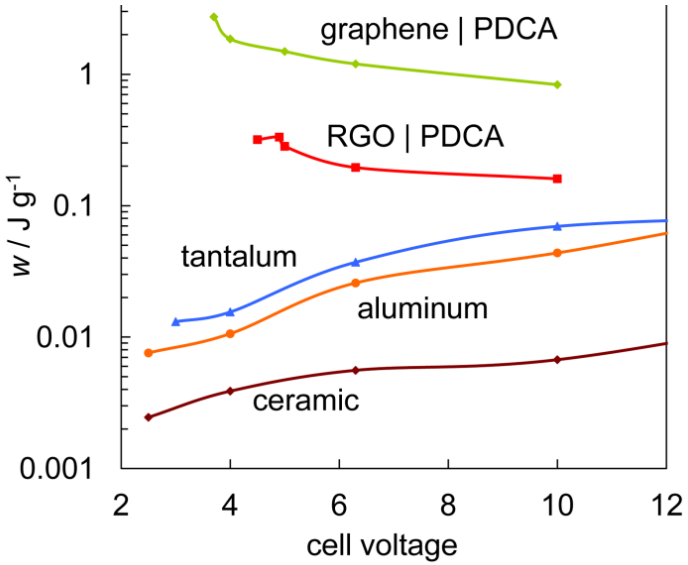
Potential calculation (gmx potential)

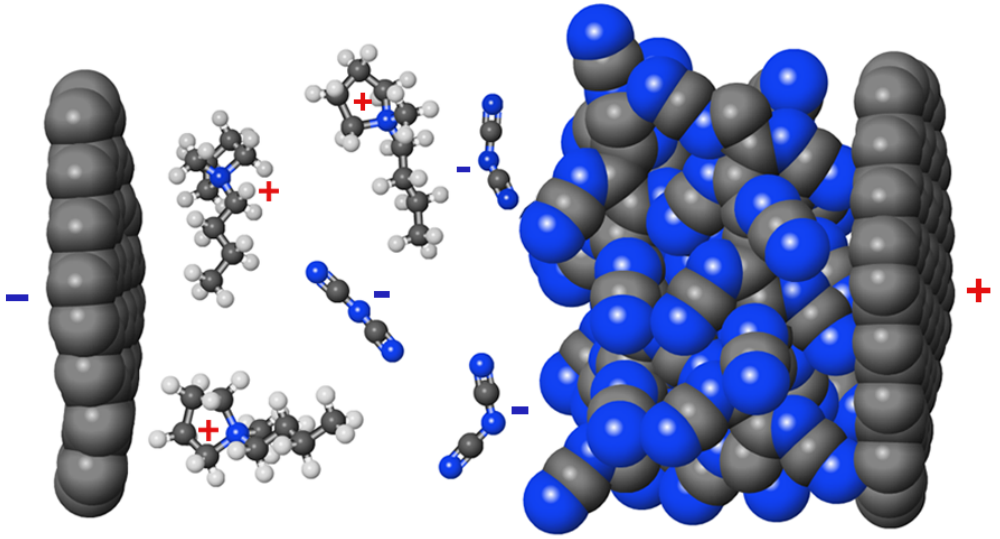
- Capacitance calculation



V. Ivaništšev, M.V. Fedorov, R.M. Lynden-Bell, J. Phys. Chem. C 118 (2014) 5841–5847.
V. Ivaništšev, K. Kirchner, *et al.*, J. Phys.: Condens. Matter 27 (2015) 102101.
V. Ivaništšev, S. O'Connor, M.V. Fedorov, Electrochem. Commun. 48 (2014) 61–64.

Novel high voltage graphene|ionic liquid capacitor technology – mesoporous RGO-based anode (50-200 um thick), RGO-based cathode (0.1-10 um thick), BMPDCA electrolyte.

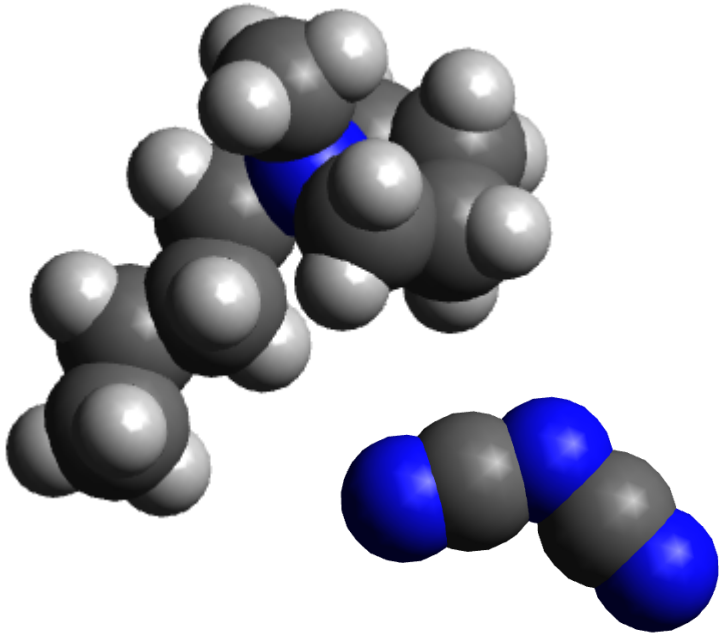




- First time voltages over 4 V for a C-C electrochemical capacitor
- 2 000 times faster than a supercapacitor.
- New polymer polydicyanamide was characterized, structure resolved.

T. Romann et al. 4-10 V capacitors with graphene-based electrodes and ionic liquid electrolyte. J. .

T. Romann, E. Lust, O. Oll, Method of forming a dielectric through electrodeposition on an electrode for a capacitor, patent , 2016.



tinyurl.com/RIGA18bulk

tinyurl.com/RIGA18wall

Thank you for your attention!