

## **Energy harvesting and storage with ionic liquids: the essential physics at the nanoscale**

Alexei A. Kornyshev

Imperial College London, SW7 2AZ UK

The renewal of interest to fundamental mechanisms of energy storage in electrochemical supercapacitors was boosted by the progress in development of novel materials (mainly carbon based) for nanostructured electrodes. It was also affected by the booming research in room temperature ionic liquids that offers virtually unlimited number of new electrolyte combinations. Some of them have large potential windows that allow to charge capacitors to higher voltages and thereby store more energy. This material-science based progress had to be matched with detailed investigation of performance of such systems. In particular, exploiting ultrananoporous electrodes, with pores just about to accommodate one layer or one row of ions, can increase the interfacial area and thereby the stored energy, but what will be the capacitance-voltage dependence and the dynamics of charging of such electrodes? What are the laws of population of such pores with ions subject to applied potential, and the conditions for maximizing stored energy and power?

There was a considerable progress in this area over the last five years. Basic mechanisms of charge equilibria in ultrananoporous electrodes have been understood based on statistical theory of ion-ion and ion interactions in nano-confinement. The modes of charging dynamics have also been revealed based on kinetic theory and simulations. The talk will overview these advances, with a focus on the effects that theory explains or predicts, as well as highlight pressing questions for future experiments and theory.

Sister systems to supercapacitors are electroactuators. These can be and are being used for the conversion of time dependent applied voltage into mechanical motion, or other way around – for the conversion of the applied force into the AC current. Such harvesters of mechanical work, draw currently attention in the context of AC-current generation from walking. Physics of this class of systems will also be briefly reviewed.

Sister problems emerge also in nanotribology, the subject related to minimizing energy losses: electrotuneable lubricity with ionic liquid lubricants which, time permitting, I will also cover.

With intention to overview this whole research area, the talk will still be majorly based on a series of joint works of *theoretical chemical physics* team at Imperial College and our partners at University of Strathclyde, University of Drexel, Virginia Tech, ORNL, FZ-Juelich, University of Tel Aviv, LPTL CNRS (France), HUST (China), and other groups, to be highlighted and acknowledged in the talk. Some papers of this series are cited below.

1. M.V.Fedorov and A.A.Kornyshev, Ionic liquids at electrified interfaces, *Chem.Rev.***114**, 2978–3036 (2014).
2. S.Kondrat, A.Kornyshev, Charging dynamics and optimization of nanoporous supercapacitors, *J.Phys.Chem.C* **117**, 12399-12406 (2013).
3. S.Kondrat, P.Wu, R.Qiao, A.A.Kornyshev, Accelerating charging dynamics in subnanometer pores, *Nature Materials* **13**, 387-393(2014).
4. Y.He, J. Huang,B.G. Sumpter, A.A.Kornyshev, R.Qiao, Dynamic charge storage in ionic liquids-filled nanopores: insight from a computational cyclic voltammetry study, *J. Phys. Chem. Lett.* 2015, **6**, 22–30 (2015).
5. A.A.Lee, S.Kondrat, G.Oshanin, A.A.Kornyshev, Charging dynamics of a supercapacitor with narrow cylindrical nanopores, *Nanotech.***25**, #315401 (2014).
6. S. Kondrat, A.A.Kornyshev, Pressing a spring: what does it take to maximize the energy storage in nanoporous supercapacitors? *Nanoscale Horizons*, **1**, 45-52 (2016).
7. A.A.Kornyshev, The simplest model of charge storage in single file metallic nanopores, *Faraday Disc.* **164**, 117-133 (2013).
8. C.C. Rochester, G.Pruessner, A.A.Kornyshev, Statistical mechanics of 'unwanted electroactuation' in nanoporous supercapacitors, [\*Electrochim.Acta\* \*\*174\*\*, 978-984 \(2015\)](#).
9. G.Feng, X.Jiang, R.Qiao, A.A.Kornyshev, Water in ionic liquids at electrified interfaces: the anatomy of electrosorption, *ACS Nano* **8**, 11685–11694 (2014).
10. A.A.Lee, S.Kondrat, A.A.Kornyshev, Single-file charge storage in conducting nanopores, *Phys.Rev.Lett.* **113**, #048701, 1-5 (2014).
11. O.Y.Fajardo, F.Bresme, A.A.Kornyshev, M.Urbakh, [Electrotunable lubricity with ionic liquid nanoscale films](#), *Sci.Rep.* **5**, 2045-2322 (2015).
12. O.Y.Fajardo, F.Bresme, A.A.Kornyshev, M.Urbakh, [Electrotunable friction with ionic liquid lubricants: how important is the molecular structure of the ions?](#), *J.Phys.Chem.Lett.* **6**, 3998-4004 (2015).
13. C.C.Rochester, S.Kondrat, G.Pruessner, A.A Kornyshev (2016), [Charging ultrananoporous electrodes with size-asymmetric ions assisted by apolar solvent](#), *J.Phys.Chem.C* **120**, 16042-16050 (2016).
14. A.A. Kornyshev, R. Twidale, A.Kolomeisky, Current generating double layer shoe with a porous sole: ion transport matters, *J.Phys.Chem.C* **121**, 7584-7595 (2017).
15. Z.A.H. Goodwin, G. Feng, A. A. Kornyshev, [Mean-field theory of electrical double layer in ionic liquids with account of short-range correlations](#), *Electrochimica Acta*, **225**,190-197 (2017).
16. O.Y.Fajardo, F.Bresme, A.A.Kornyshev, M.Urbakh, Water in ionic liquid lubricants: friend and foe, *ACS Nano*, **11**, 6825-6831 (2017).