Extreme Scale Computational Nanoscience and Engineering for Exploring and Optimizing Energy Storage and Conversion

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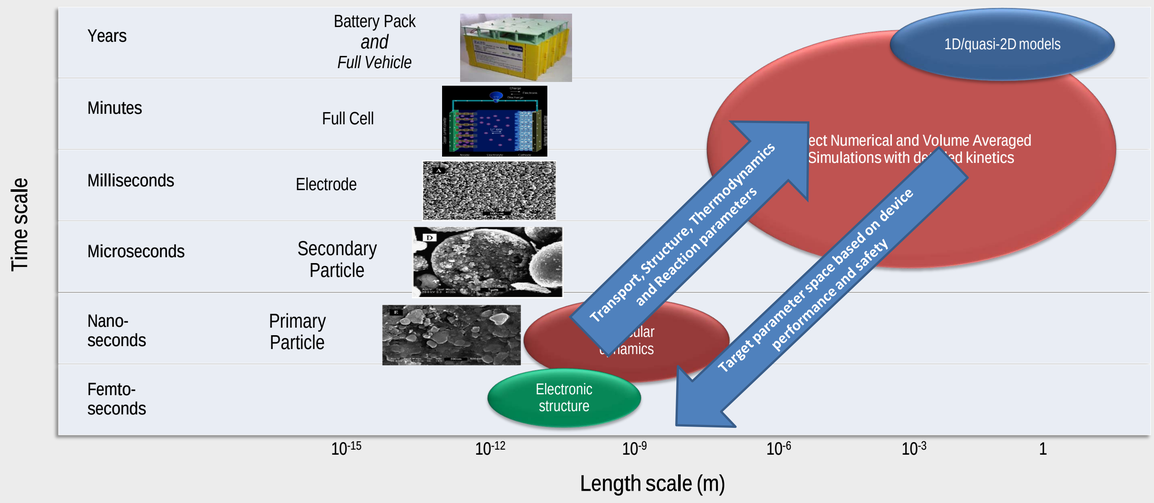
Background

Efficient, flexible, and safe electrical energy torage technology is one of the fundamental elements to reducing our dependency on fossil fuels and diversifying our energy sources. Electrochemical energy storage devices (batteries and supercapacitors) are the leading candidates for meeting our current and future electrical energy storage needs. Both types of electrochemical energy storage devices critically need improved quantitative understanding of the underlying electrochemical processes in order to enhance their performance.

Improved capability for energy conversion are also desperately needed. In particular with respect to our current ability to "harvest" energy from the sun (solar fuels or solar photovoltaics).

Size and Time Scale



Exascale computing can be a critical part of enabling accurate and efficient simulation for energy science

Theory and modeling for Energy Storage Materials

Helmholtz and post-Helmholtz models

EDLC

$C = \varepsilon_r\varepsilon_0 A/d$ (1a)

$C/A = \varepsilon_r\varepsilon_0/d$ (1b)

The traditional Helmholtz model has been used for decades. New materials call for new post-Helmholtz models.

EDCC

$C = 2\pi\varepsilon_r\varepsilon_0 L / \ln(b/a)$ (2a)

$C/A = \varepsilon_r\varepsilon_0/\{b\ln[b/(b-d)]\}$ (2b)

xEDSC

$C = 4\pi\varepsilon_r\varepsilon_0 ab/(b-a)$ (4a)

$C/A = \varepsilon_r\varepsilon_0(a+d)/ad$ (4b)

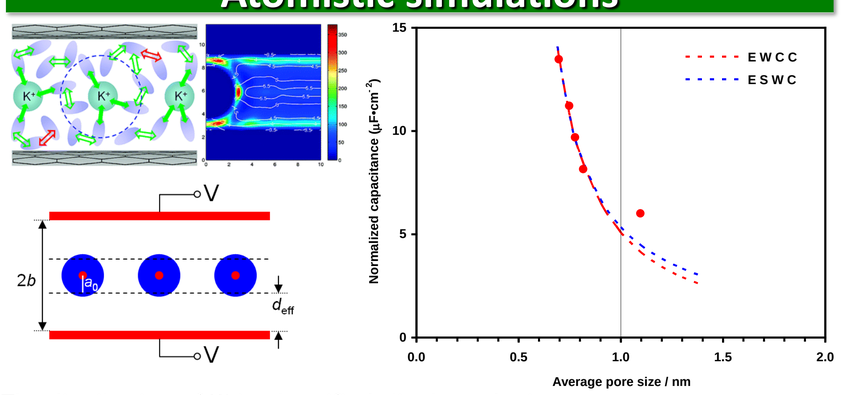
EWCC

$C/A = \varepsilon_r\varepsilon_0/[b\ln(b/a_0)]$ (3)

xEDCC

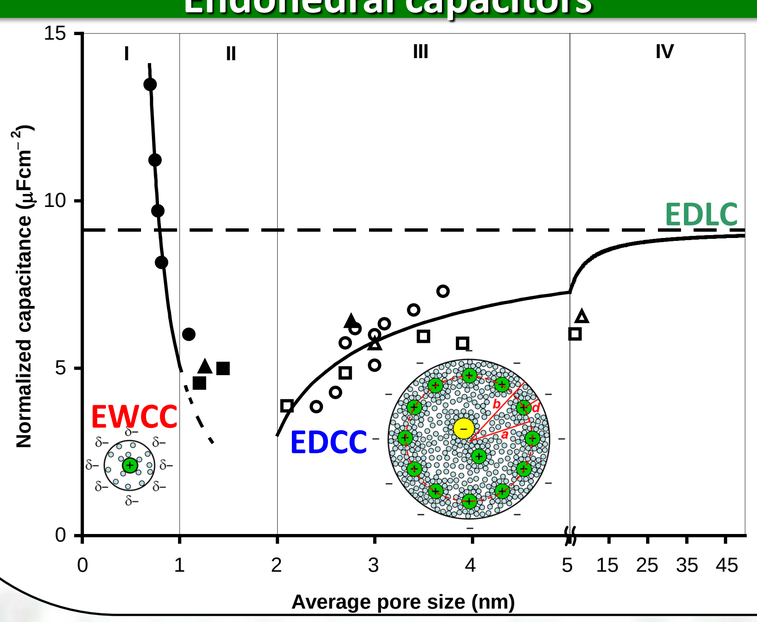
$C/A = \varepsilon_r\varepsilon_0/\{a\ln[(a+d)/a]\}$ (5)

Atomistic simulations

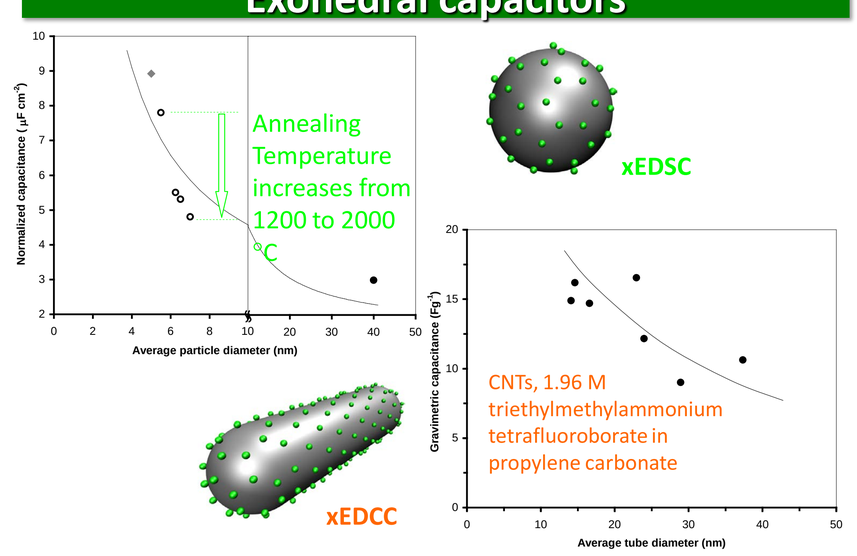


The distribution of K^+ in electrified slit-shaped micropores
MD simulations. For pore widths b/w 10 and 14.7 Å, fully hydrated ions

Endohedral capacitors

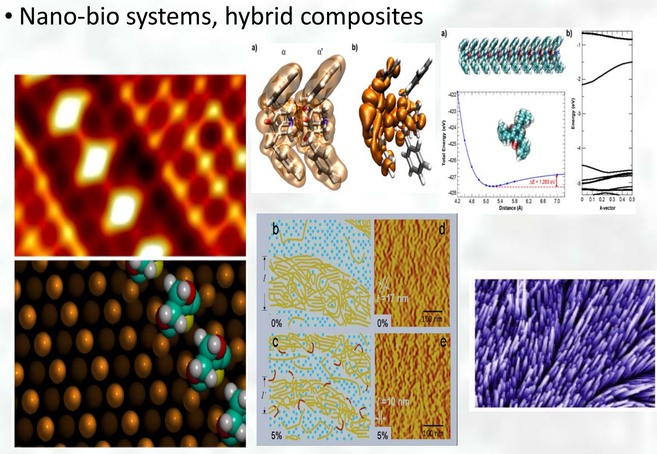


Exohedral capacitors



How can we control long-range supramolecular ordering?

- Epitaxially confined arrays of conjugated polymeric materials
- Processing using controlled annealing, compatibilizers, substrate
- Alternative organic systems such as crystalline organic nanowires
- Nano-bio systems, hybrid composites



PNAS, 107, 11200 (2010); Science 323, 1701 (2009); J. Phys. Chem. C. 111,18912 (2007);PNAS 106, 4591 (2009); Nano Lett. 9, 1487 (2009); PRL 105, 045501 (2010)

Conclusions

Theory, modeling, and simulation of materials provides essential information to enable fundamental understanding of the role of pore size, shape, and self-assembly in energy storage and conversion processes.

Acknowledgements

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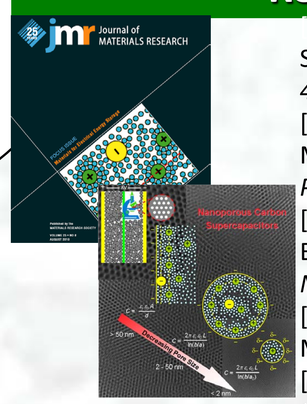

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