CAMBRIDGE ZERO$_2$

Energy Materials
Special Interest Group

Cambridge Energy Materials Research Seminar
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Panel

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Challenges

- Increasing energy density of supercapacitors.
- Understanding the charge storage mechanism of supercapacitors.
- Identifying measurable properties which correlate with supercapacitor energy storage properties.
- Computational modelling of complex systems containing water, such as water splitting systems, aqueous supercapacitors, and aqueous batteries.
- Ab initio calculations are accurate but slow, while force field calculations are fast but inaccurate.

Discussion Points

- Supercapacitors are cheap, fast-charging and durable energy storage devices used in systems which require high energy densities and fast response times, such as electric buses. They are promising for other applications such as grid storage and stabilisation but use for these purposes is held back by a low charge storage capacity relative to lithium-ion batteries or equivalent technologies.
- Development of supercapacitors with higher energy storage capacity has been limited by an unclear mechanism of action, making device optimisation difficult. An outstanding question in the field is how the structure of the porous activated carbon electrode affects the capacity.
- Spectroscopic methods have identified that a higher structural disorder of the activated carbon results in better energy storage properties. Measurement of disorder can be achieved quickly with either NMR or Raman spectroscopy.
- Reactivities and interactions of water are key parameters for many systems of interest in energy materials, including supercapacitors, batteries, and water splitting systems.
- Computationally modelling water systems requires simulating thermodynamic, structural, and dynamical properties of the system, with small changes to computational methods causing diverging results.
- Machine learning computational methods, such as the recently developed MACE model, combine the advantages of ab initio and forcefield methods, enabling accurate and computationally efficient simulation of systems containing large numbers of water molecules.
- These methods are data-driven, can probe reactivity, and with enough training can be brought to whatever level of accuracy is required for the problem at hand.
- Systems of interest for ongoing research include heterogenous zeolite catalysts, reactions between CO_2 and water at gas: liquid interfaces, and water: ion interactions in battery and supercapacitor electrolytes, studying properties such as proton diffusion.

Opportunities

- Higher-capacity supercapacitors could offer an alternative to batteries when fast charging and long-term stability are important, though both technologies will continue to coexist.
- New spectroscopic methods for measuring disorder will allow rapid screening of electrode materials for improved supercapacitors, guided by an improved understanding of the mechanism of supercapacitor charge storage.
- Improved modelling techniques allow modelling of many more structures and materials than was previously possible.
- Large water-containing systems are particularly approachable with the MACE model compared to previously available methods.

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