Comp. Mat. Sci. for Energy & Environment

Keywords: Interface, battery, cell, catalyst, electrochemistry, first-principles calc., sampling

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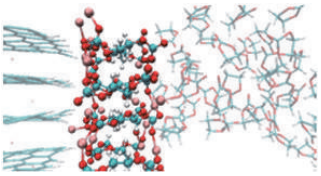
Background

- Several long-standing issues in battery and catalyst science.
- Less understanding of interfacial redox reactions on the atomic scale.
- Developing interface science for energy & environmental processes.

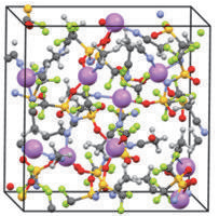
Aim

- Computational predictions of interfacial phenomena difficult to be observed.
- Theoretical / computational developments for interfacial redox reactions.
- Establishment of interface science for energy & environmental processes.

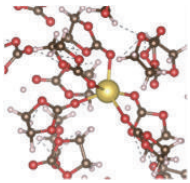
Advanced Research Topics



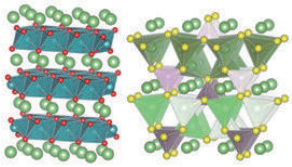
Battery: SEI film mechanism



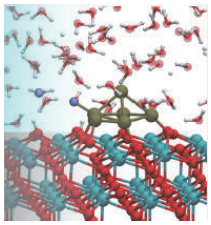
Battery: highly concentrated electrolyte



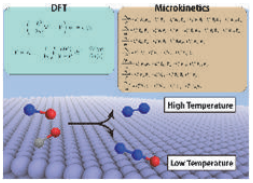
Battery: solvation / desolvation



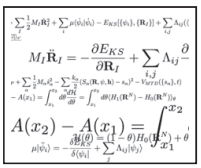
Battery (solid-state): interfacial resistance



Catalyst: metal supported oxide / water interface



Catalyst: first-principles surface microkinetics for multi-scale calc.



Method: Efficient code for first-principles free energy calc.

Publications

・Battery interfaces (liquid/solid electrolytes) : JACS 135, 11967 (2013), Chem. Mater. 26, 4248 (2014). JES 162, A2670 (2015), PCCP 18, 8643 (2016), ACS-AMI 9, 286 (2017).
・Batttery highly-concentrated electrolytes: JACS 136, 5039 (2014), JPCC 118, 14091 (2014), Nat. Commun. 7, 12032 (2016), Nat. Energy 1, 16129 (2016), ACS-AMI 9, 33802 (2017), Nat. Energy 3, 22 (2018).
・Catalysts: JPCC 118, 22040 (2014), JPCC 119, 2537 (2015), JACS 139, 11570 (2016), JPCC 122,17378 (2018).
・Solar cell: JPCC 118, 16863 (2014), JPCL 5, 2903 (2014), JACS 137, 10048 (2015), ACR 49, 554 (2016), JPCL 8, 5840 (2017).
・Methodology: PCCP 16, 19530 (2014), PCCP 17, 27103 (2015), Sci. Rep. 5, 18220 (2015).

Summary

- Solving long-standing issues in battery and catalyst science
- Proposal of new concepts such as highly concentrated electrolyte
- New computational / theoretical tools

Research outcome

- Development of next-geneation batteries
- Development of novel catalysts
- Protocol for high performance computing of materials science issues