WWU MÜNSTER

Theoretical Description of Electrochemical Processes

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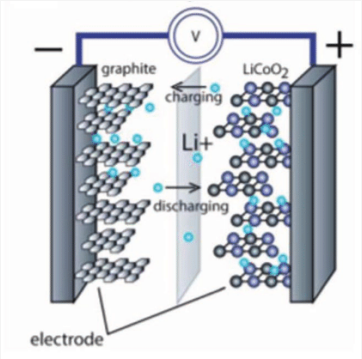
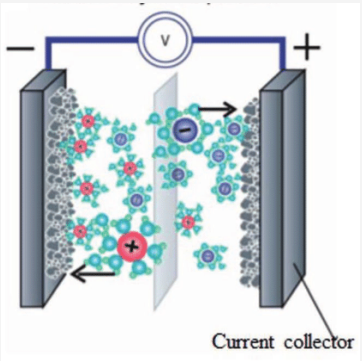
CMTC Center for Multiscale Theory and Computation

Ionics – Electrostatics at Interfaces

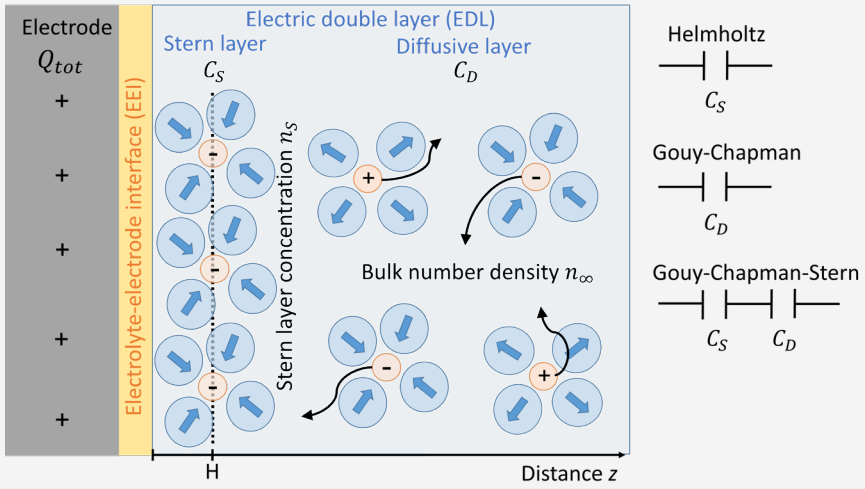


Li-ion batteries

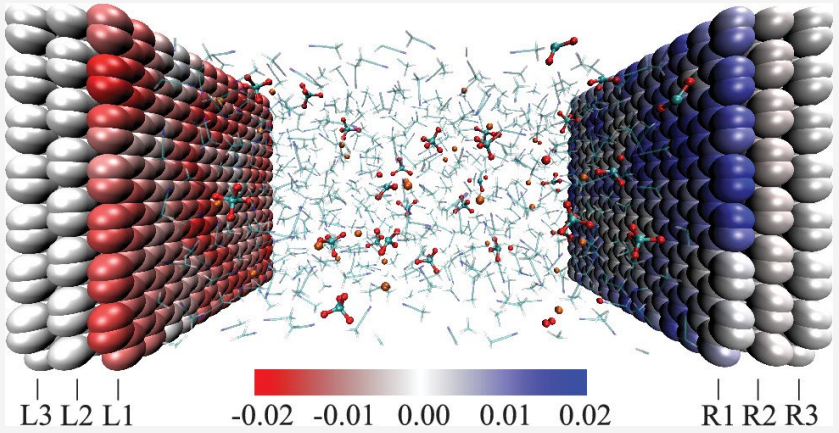


Supercaps

Analytical models



Simulation approaches

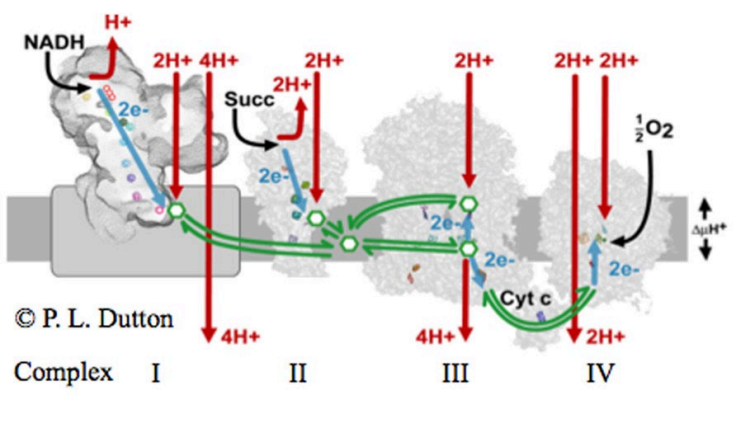


How to model charged electrodes in MD simulations?

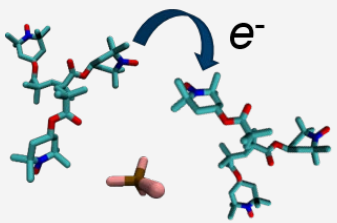
- constant charge
- image charges
- constant voltage

[1] Jost *et al.*, *J. Mater. Chem. A* **2**, 10776-10787 (2014)
[2] Wang *et al.*, *J. Chem. Phys.* **141**, 184102 (2014)

Electronics – Modeling Electron Transfer Processes

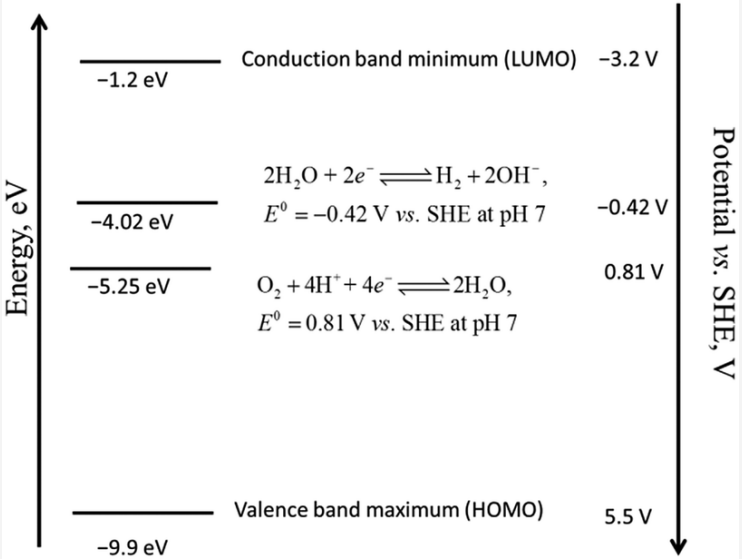


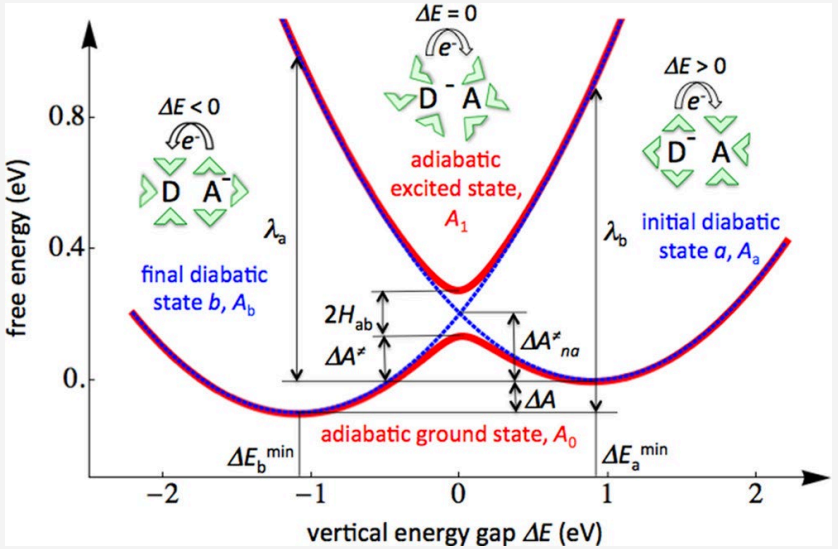
- Batteries, fuel cells, catalysis
- (Conductive) polymers
- Biological systems (e.g. aerobic respiration, photosynthesis)



Analytical models

- Marcus theory
- Butler-Volmer equation
- Electrochemical reactions





Modeling approaches

- cDFT, TD-DFT, CASSCF, FMO
- Classical MD (impact of intermolecular environment)

[1]

[1] Blumberger, *Chem. Rev.* **115**, 20, 11191 (2015)
[2] Peljo *et al.*, *Energy Environ. Sci.* **11**, 2306-2309 (2018)

Mögliche Termine (Abstimmung mit Teilnehmenden)

1 SWS, ca. 7 Termine

Mögliche Zeiträume, auch als Blockseminar:

Montags (08:00 – 12:00)

Mittwochs (15:00 – 17:00)

Donnerstags (08:00 – 12:00)

Freitags (08:00-10:00; 12:00-16:00)