Physikalisches Institut
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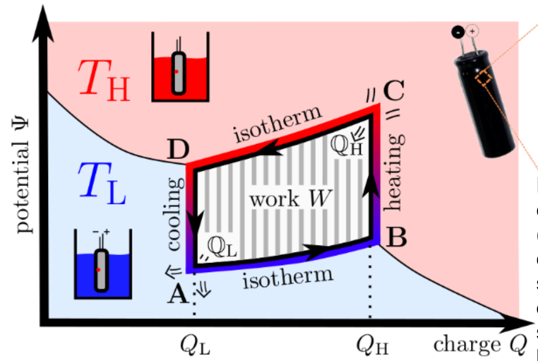

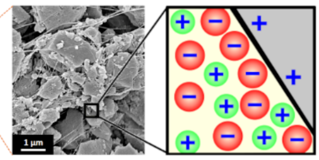

Figure 1. Thermocapacitive cycle using a supercapacitor (left) and zoom into a porous carbon electrode of the supercapacitor (right). The electrolyte at the electrode's surface forms the electric double layer. Figure reproduced from [Energy Environ. Sci. **8**, 2396 (2015)]

UNDERSCREENING, OVERSCREENING, AND BLUE ENERGY – HOW ELECTROSTATIC INTERACTIONS CAN BE EXPLOITED IN A THERMODYNAMIC ENGINE FOR SUSTAINABLE ENERGY CONVERSION

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The efficient storage of energy and the reuse of waste heat are important processes to tackle climate change. Interestingly, supercapacitive energy-storage devices not only allow to store electric energy, but their physical functionality also allows to exploit the charging process itself within novel thermodynamic cycles. These cycles allow to harvest so-called Blue Energy from salinity steps and from waste heat. I will demonstrate how such cycles can be designed and that classical density functional theory allows to explicitly calculate them. In particular, I will discuss the physics of socalled electric double layers (see Figure 1), those regions next to the electrodes of a capacitor where the mobile charges in the electrolyte arrange themselves to screen the electrode's electrostatic field. At sufficiently low ionic concentration, electric double layers are well described by Poisson-Boltzmann theories, which approximate ions by point-like particles. At higher concentrations, however, ionic sizes are non negligible. Steric effects then lead to over- or underscreening, respectively corresponding to a more or less efficient screening compared to what expected for point-like ions. Underscreening has only recently been discovered in experimental measurements and no clear consensus has been reached between experiments and theoretical descriptions since then. Based on density functional theory and computer simulations of a primitive ion model, I will present a consistent picture of underscreening that challenges our current understanding of dense electrolytes. A deep understanding of electrostatic screening in general can lead to an optimization of charging and energy harvesting. This, finally, will contribute to a more sustainable use of energy.

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