



# "Soft-Matter Seminar"

## „Monte Carlo simulation of electrolytes in the constant voltage ensemble"

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### Abstract:

Monte Carlo simulation studies on electrolytes near electrodes are often performed with a constant surface charge density on the electrodes. In most electrochemical experiments, however, the voltage is kept constant rather than the surface charge density. We have developed a technique to perform a Monte Carlo simulation in the constant voltage ensemble, in which the chemical potential difference of electrons between the cathode and the anode is kept constant. In this ensemble, the electrochemical properties such as the electrical potential profile and the capacitance are calculated in a more natural fashion than in the ensemble with a constant surface charge density. Application of this technique to planar and porous electrodes will be discussed.

**Mittwoch, den 16.9.2009**  
**14:00 Uhr**  
**Raum PH 3344**

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