Screening of Charged Electrodes by Ionic Liquids: A Simulation Study

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Frontiers in Chemical Physics
Seminar Series

Presented by…

Ruth Lynden-Bell

Professor, Department of Chemistry
University of Cambridge, UK

Near a solid wall ionic liquids are layers. If the walls are charged, layers of cations and anions tend to separate, due to electrostatic forces. Although the average charge density is zero in the bulk of the liquid, near the walls there are large oscillations in the charge density and potential as a function of distance from the wall. There is significant overcompensation of the wall charge by the first liquid layer, which is reversed in the second layer. Measurements of free energy profiles show that charged solutes prefer to embed themselves in layers of the same charge, replacing ionic liquid ions. This results in high free energy barriers impeding the passage of charged solutes to the electrode, which may slow electrode reactions. We investigated the local environment of solute ions in regions of maximum and minimum free energy.

More info?

http://www-jmg.ch.cam.ac.uk/oldchem/staff/rmlb.html

Thursday,
September 5

EMSL Auditorium

10 – 11:30 am