

## **Charge Inversion Phenomenon in Electrolyte Liquid: Electrophoresis Study by Molecular Dynamics Simulations**

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Correlation effects in the charged particle system can cause charge inversion due to "overscreening" unlike traditional Debye screening. For the phenomenon to take place, two conditions need to be met: Counterions are multivalently charged and Coulomb interactions are strong enough compared to thermal energy [1]. We have performed molecular dynamics simulations of the (overall neutral) system consisting of a macroion and the electrolyte of counterions and coions, where solvent neutral particles are simulated along with ions. Under an external electric field, the macroion drifts together with the strongly adsorbed multivalent counterions along the electric field, in the direction proving inversion of the charge sign [2]. The reversed mobility of the macroion is insensitive to the external field, which increases with salt ionic strength and counterion valence. The motion of the macroion complex does not induce any flow of the neutral solvent away from the macroion, which reveals screening of hydrodynamic interactions at short distances in electrolyte liquid. A very large electric field, comparable to the macroion unscreened field, disrupts charge inversion by stripping the adsorbed counterions off the macroion.

### **References:**

- [1] M.Tanaka and A.Yu.Grosberg, J.Chem.Phys. 115, 567 (2001).
- [2] M.Tanaka and A.Yu.Grosberg, Euro.Phys.J., E7, 371 (2002).

The present computation was performed using Origin 3800 of the Minnesota Supercomputing Institute and vpp800/12 of the National Institute for Space and Astronautical Science of Japan.