

Charge Inversion of a Weakly Charged Macroion in Sphere/Rod Shapes: Effects of Anions, Salt, and Polymer Cations¹ MOTOHIKO TANAKA, National Institute for Fusion Science, Toki 509-5292, Japan, ALEXANDER YU. GROESBERG, Physics Department, University of Minnesota, Minneapolis, MN55455 — We have studied by molecular dynamics simulations the charge inversion process of a weakly charged macroion in sphere/rod shapes like DNA, focusing on the effects of coions, salt, and polymer counterions. The reversed electrophoretic mobility increases with the ratio of coion to counterion radii, while it decreases with the coion to counterion valences Z^-/Z^+ which becomes non-reversed for $Z^- > Z^+$. The monovalent salt suppresses reversed mobility when its ionic strength exceeds that of the adsorbed counterions, except for mobility enhancement of a strongly charged macroion at small salt ionic strengths. There is a threshold surface charge density for charge inversion to take place. Polymer counterions made of multivalent ions are effective for getting a weakly charged macroion like DNA charge inverted, with the help of large coions and short-range adhesive forces. The mobility of an elongated macroion can further be enhanced by mechanical twining of charged polymers around the long axis.

¹This study was performed using Origin3800 of the University of Minnesota Supercomputing Institute, and vpp800/13 of Institute of Space and Astronautical Science (Japan).