Accepted Manuscript

Measuring surface charge: Why experimental characterization and molecular modeling should be coupled

Remco Hartkamp, Anne-Laure Biance, Li Fu, Jean-François Dufrêche, Oriane Bonhomme, Laurent Joly

PII: S1359-0294(18)30005-0
DOI: doi:10.1016/j.cocis.2018.08.001
Reference: COCIS 1210

To appear in: *Current Opinion in Colloid & Interface Science*

Received date: 31 March 2018
Revised date: 10 July 2018
Accepted date: 3 August 2018

Please cite this article as: Remco Hartkamp, Anne-Laure Biance, Li Fu, Jean-François Dufrêche, Oriane Bonhomme, Laurent Joly , Measuring surface charge: Why experimental characterization and molecular modeling should be coupled. Cocis (2018), doi:10.1016/j.cocis.2018.08.001

Current Opinion in Colloid and Interface Science

Measuring surface charge: why experimental characterization and molecular modeling should be coupled

Remco Hartkamp, Anne-Laure Biance, Li Fu, Jean-François Dufrêche, Oriane Bonhomme[1], Laurent Joly

Process & Energy Department, Delft University of Technology, Leeghwaterstraat 39, 2628 CB Delft, The Netherlands
Univ Lyon, Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, F-69622 Villeurbanne, France
Institut de Chimie Séparative de Marcoule ICSM, UMR 5257
CEA-CNRS-ENSCM-Université Montpellier, Bâtiment 426, F-30207 Bagnols-sur-Cèze, France

Abstract

Surface charge controls many static and dynamic properties of soft matter and micro/nanofluidic systems, but its unambiguous measurement forms a challenge. Standard characterization methods typically probe an effective surface charge, which provides limited insight into the distribution and dynamics of charge across the interface, and which cannot predict consistently all surface-charge-governed properties. New experimental approaches provide local information on both structure and transport, but models are typically required to interpret raw data. Conversely, molecular dynamics simulations have helped showing the limits of standard models and developing more accurate ones, but their reliability is limited by the empirical interaction potentials they are usually based on. This review highlights recent developments and limitations in both experimental and computational research focusing on the liquid-solid interface. Based on recent studies, we make the case that coupling of experiments and simulations is pivotal tomitigate methodological shortcomings and address open problems pertaining to charged interfaces.

surface charge, electrical double layer, zeta potential, electrokinetics, scanning probe microscopy, spectroscopy, molecular dynamics, ab initio methods

1. Introduction

When a solid surface meets an aqueous electrolyte, physical or chemical mechanisms can generate an electric surface charge [1,2,3,4]. Ions in the liquid reorganize to form a nanometric layer to balancethe surface charge, the electrical double layer (EDL). Surface charge governs the stability and dynamics of soft matter systems, and as such it is a key property to characterize. Surface charge also drives the response of nanofluidic systems to thermodynamic gradients [5]. The development of new membranes to harvest e.g. blue energy (the osmotic energy of sea water) [6,7,8] has led to a renewed interest for finding new functional interfaces with optimal surface charge.

[1]*Email Addresses:* oriane.bonhomme@univ-lyon1.fr (Oriane Bonhomme), laurent.joly@univ-lyon1.fr (Laurent Joly)