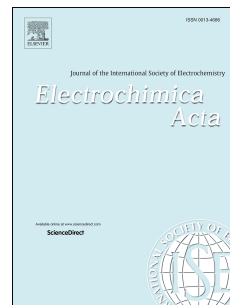


# Accepted Manuscript

Theory of electrosorption of water from ionic liquids

Yury A. Budkov, Andrei L. Kolesnikov, Zachary A.H. Goodwin, Mikhail G. Kiselev,  
Alexei A. Kornyshev



PII: S0013-4686(18)31653-0

DOI: [10.1016/j.electacta.2018.07.139](https://doi.org/10.1016/j.electacta.2018.07.139)

Reference: EA 32336

To appear in: *Electrochimica Acta*

Received Date: 10 April 2018

Revised Date: 25 June 2018

Accepted Date: 19 July 2018

Please cite this article as: Y.A. Budkov, A.L. Kolesnikov, Z.A.H. Goodwin, M.G. Kiselev, A.A. Kornyshev, Theory of electrosorption of water from ionic liquids, *Electrochimica Acta* (2018), doi: 10.1016/j.electacta.2018.07.139.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

# Theory of Electrosorption of Water from Ionic Liquids

Yury A. Budkov<sup>a,b</sup>, Andrei L. Kolesnikov<sup>c,d</sup>, Zachary A.H. Goodwin<sup>e,f</sup>,  
Mikhail G. Kiselev<sup>b</sup>, Alexei A. Kornyshev<sup>f,1</sup>

<sup>a</sup>*Tikhonov Moscow Institute of Electronics and Mathematics, School of Applied Mathematics, National Research University Higher School of Economics, 34 Tallinskaya Ulitsa, 123458, Moscow, Russia*

<sup>b</sup>*G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences, Laboratory of NMR spectroscopy and numerical investigations of liquids, Ivanovo, Russia*

<sup>c</sup>*Porotec GmbH, Niederhofheimer Str. 55 A, 65719 Hofheim am Taunus, Germany*

<sup>d</sup>*Institut für Nichtklassische Chemie e.V., Permoserstr. 15, 04318 Leipzig, Germany*

<sup>e</sup>*Imperial College London, Department of Physics, CDT TSM, Imperial College Rd, London, SW72AZ, United Kingdom*

<sup>f</sup>*Imperial College London, Department of Chemistry, Imperial College Rd, London, SW72AZ, United Kingdom*

---

## Abstract

We propose and develop a classical density functional theory for the description of a minor amount of water dissolved in ionic liquid in the vicinity of an electrode. In addition to the electrostatic energy and lattice-gas mixing entropy terms, the utilised grand canonical potential contains several phenomenological terms/parameters that describe short-range interactions between ions of ionic liquid, water molecules and the electrode. Some of these have been earlier introduced in the theory of electrical double layer in pure ionic liquids. Based on this, we investigate the role of the remaining 'specific interaction' parameters – those that characterize possible (i) specific interaction of ions and molecules with the electrode, which are responsible for their specific adsorption; and (ii) hydrophilicity/hydrophobicity of ions. As a result we obtain water electrosorption isotherms as a function of the potential drop across the electrical double layer, investigate its asymmetry with respect to the sign of electrode potential, and establish the relationship between the sign of this asymmetry and hydrophobicity/hydrophilicity of cations and anions. We also calculate the effect of water electrosorption on the double layer differential capacitance which brings clear new features

---

<sup>1</sup>a.kornyshev@imperial.ac.uk

Download English Version:

<https://daneshyari.com/en/article/6601949>

Download Persian Version:

<https://daneshyari.com/article/6601949>

[Daneshyari.com](https://daneshyari.com)