On the temperature dependence of the double layer capacitance of ionic liquids

Ming Chen, Zachary A.H. Goodwin, Guang Feng, Alexei A. Kornyshev

PII: S1572-6657(17)30783-X
DOI: doi: 10.1016/j.jelechem.2017.11.005
Reference: JEAC 3635

To appear in: *Journal of Electroanalytical Chemistry*

Received date: 20 September 2017
Revised date: 1 November 2017
Accepted date: 2 November 2017

Please cite this article as: Ming Chen, Zachary A.H. Goodwin, Guang Feng, Alexei A. Kornyshev, On the temperature dependence of the double layer capacitance of ionic liquids, *Journal of Electroanalytical Chemistry* (2017), doi: 10.1016/j.jelechem.2017.11.005

On the Temperature Dependence of the Double Layer Capacitance of Ionic Liquids[†]

Ming Chen[a], Zachary A. H. Goodwin[b,c], Guang Feng[a], Alexei A. Kornyshev[a,b,*]

[a] *State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology (HUST), Wuhan 430074, China*
[b] *Imperial College London, Department of Chemistry, Imperial College Rd, London, SW7 2AZ*
[c] *Imperial College London, Department of Physics, Imperial College Rd, London, SW7 2AZ*

Abstract

The temperature dependence of room temperature ionic liquids differential capacitance is studied here with both theoretical and computational methods. On the theory aspect, the lattice-gas mean-field theory of ionic liquids is further generalised to account for 'ion pairing' and 'neutral aggregate' formation. An anomalous temperature dependence of linear response capacitance was found, similar to that of earlier work. The theory also predicted that differential capacitance curves transform from a camel to bell shape with increasing temperature. Molecular dynamics simulations verified the expected transition in shape of differential capacitance curves with temperature and the dependence of linear response capacitance on temperature. Further investigation into charge density distributions revealed an ordered structure, reminiscent of oriented ion pairs and neutral aggregates, extending far enough from the electrode to control the capacitance-voltage response. It was found that these structures were dismantled with increasing temperature, as predicted by the mean-field theory.

Keywords: room temperature ionic liquids, mean-field, temperature,

*Corresponding author
Email address: a.kornyshev@imperial.ac.uk (Alexei A. Kornyshev)

[†] This paper is devoted to the memory of an outstanding electrochemist, and great personality, Roger Parsons, whom one of us (AAK) closely knew and whose contributions to understanding the electrical double layer influenced many researches.