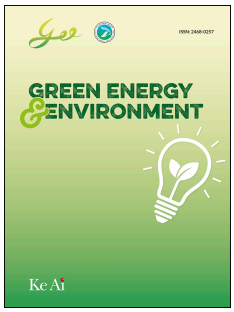
Accepted Manuscript



Molecular Dynamics Study of Room Temperature Ionic Liquids with Water at Mica Surface

Huanhuan Zhang, Mengyang Zhu, Zhao Wei, Song Li, Guang Feng

PII: S2468-0257(17)30133-4

DOI: 10.1016/j.gee.2017.11.002

Reference: GEE 96

To appear in: *Green Energy and Environment*

Received Date: 6 August 2017

Revised Date: 10 November 2017

Accepted Date: 27 November 2017

Please cite this article as: H. Zhang, M. Zhu, Z. Wei, S. Li, G. Feng, Molecular Dynamics Study of Room Temperature Ionic Liquids with Water at Mica Surface, *Green Energy & Environment* (2018), doi: 10.1016/j.gee.2017.11.002.

Molecular Dynamics Study of Room Temperature Ionic Liquids with Water at Mica Surface

Huanhuan Zhang[a], Mengyang Zhu[b], Zhao Wei[a], Song Li[a,c], Guang Feng[a,c]

[a]*State Key Laboratory of Coal Combustion, School of Energy and Power Engineering, Huazhong University of Science and Technology (HUST), Wuhan 430074, China*

[b]*National Supercomputing Centre in Shenzhen, Nanshan District，Shenzhen, 518055, China*

[c]*Shenzhen Research Institute of Huazhong University of Science and Technology, Shenzhen, 518057, China*

Corresponding Author：gfeng@hust.edu.cn

Abstract

Water in room temperature ionic liquids (RTILs) could impose significant effects on their interfacial properties at a charged surface. Although the interfaces between RTILs and mica surfaces exhibit rich microstructure, the influence of water content on such interfaces is little understood, in particular, considering the fact that RTILs are always associated with water due to their hygroscopicity. In this work, we studied how different types of RTILs and different amounts of water molecules affect the RTIL-mica interfaces, especially the water distribution at mica surfaces, using molecular dynamics (MD) simulation. MD results showed that (1) there is more water and a thicker water layer adsorbed on the mica surface as the water content increases, and correspondingly the average location of K^+ ions is farther from mica surface; (2) more water accumulated at the interface with the hydrophobic [Emim][TFSI] than in case of the hydrophilic [Emim][BF_4] due to the respective RTIL hydrophobicity and ion size. A similar trend was also observed in the hydrogen bonds formed by water-water. Moreover, the 2D number density map of adsorbed water revealed that the high-density areas of water seem to be related to K^+ ions and silicon/aluminum atoms on mica surface. These results are of great importance to understand the effects of hydrophobicity/hydrophicility of RTIL and water on the interfacial microstructure at electrified surfaces.

Keywords: Room temperature ionic liquids, hydrophobicity/hydrophicility, water content, electrical double layer, mica surface