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Tarbiat Modares University

Electrochemical Society of Iran
ECSI
انجمن الکتروشیمی ایران
شماره ثبت: ۱۸۲۸۶

Certificate of Attendance

Its to certify that Mr./ Ms

Behnoosh Sadeghi

participated in 11th Annual Electrochemistry Seminar of Iran, by presenting a paper entitled:

Molecular Dynamic Study of [EMIM]+[PF6]- Ionic Liquid near a Monolayer Graphene Surface

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Molecular Dynamic Study of $[EMIM]^+[PF_6]^-$ Ionic Liquid near a Monolayer Graphene Surface

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Introduction

One of the important applications of ionic liquids is energy storage as an electric double-layer (EDL) supercapacitor. Several theoretical studies have been reported on the mechanism of EDL supercapacitors [1, 2, 3]; however, understanding molecular structure of ILs near an electrode surface is missing. In this study, detailed molecular dynamics (MD) simulation results of the structure of $[EMIM]^+[PF_6]^-$ IL near a neutral monolayer graphene electrode have been investigated.

Method and Simulation Details

All MD simulations were carried out by DL_POLY_2.17 package. An NVT ensemble at 873 K using Nose-Hoover thermostat was accomplished. To be ensured that system reaches equilibrium a three-step 1.5 ns cooling procedure, was applied on the target system. Finally, 2 ns production run was performed at 373 K and atmospheric pressure, with 1 fs time step, and 12 Å cutoff distance.

Results and Discussion

The results of MD simulation have shown accumulation of IL ions near the surface as Fig. 1 demonstrates. This aggregation has a solid like behavior over 19 Å distance away from electrode showing a layer-by-layer structure as Vatamanu et al. [2] mentioned. Number density profile of $[EMIM]^+$ cation, $[PF_6]^-$ anion, and IL shows layering structure accurately.

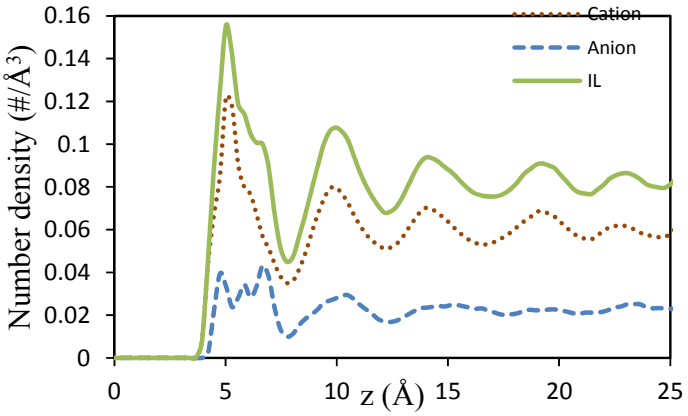

Figure 5: Number density of sum of atoms from the surface to the bulk of IL

$[EMIM]^+[PF_6]^-$ angle distribution of the first layer of imidazolium ring in Fig. 2 illustrates the cations with lower distance and more distance to the surface, were parallel and perpendicular, respectively.

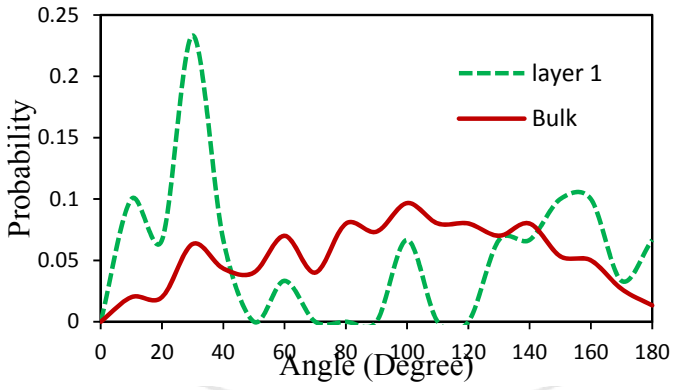

Figure 6: Angle distribution of first layer and the bulk of IL

Imidazolium charge distribution of ions was considered as a candidate of potential zero charge (PZC), to understand the charge behavior

of IL near the surface, (Fig. 3). The sharp peaks of total charge distribution tend to negative values because of the higher charge density of anions than the cations.

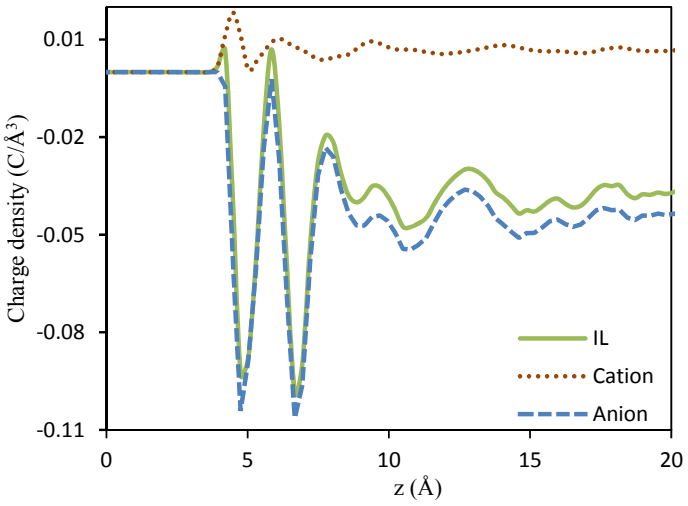

Figure 7: Charge density of cation, anion, and IL near the surface to the bulk

Conclusion

The layering behavior of $[EMIm]^+[PF_6]^-$ and total charge distribution of ions near the surface were shown the promising application of IL as supercapacitor electrolyte. It was resulted from the low charge distribution of the first layer due to its low potential zero charge.

Keywords: *Molecular Dynamics, Double Layer, Supercapacitor*

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