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Structuring, dynamics, electric double layer formation at ionic liquid/ electrode interfaces analyzed by electrochemical frequency modulation AFM and MD calculation

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Ionic liquids (ILs) are promising electrolytes for electrochemical devices such as secondary battery, capacitor, electric double layer (EDL)-FET, etc., due to their high chemical stability with negligible vaporization. Structuring, dynamics, and electric double layer formation of the interfacial IL faced to a graphite electrode or organic semiconductor surfaces were analyzed by electrochemical frequency modulation AFM (EC-FM-AFM) and molecular dynamics (MD) calculations.

MD calculations showed that layered structure of IL (BMI-TFSI) with more preference of cation to the surface was formed even at a neutral graphite, instead, the same IL formed greatly softened interface with higher mobility of ions on organic semiconductor crystal such as rubrene, which qualitatively explained our previous report on the interface evaluations using EC-FM-AFM (Fig. 1) [1-3]. The origin of the interfacial structure will be discussed based on the analyses of the local density, orientation, interaction of each ions at the interfaces including the result on a C60 crystal surface. Negatively charged graphite surfaces resulted in higher concentration of cations faced to the graphite and the effect of the structure was extended to a few nm range (Fig.2). In contrast, preference of anion at positively charged graphite surfaces was not so apparent (Fig.2). It indicates the interface structure does not symmetrically respond against the applied voltage.

Importance of the structure and flexibility of the interfacial IL on the performance of organic semiconductor based EDL-FET will also be discussed [4].

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