Electronic Supplementary Information for

Structural and dynamic properties of 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide / mica and graphite interfaces revealed by molecular dynamics simulation

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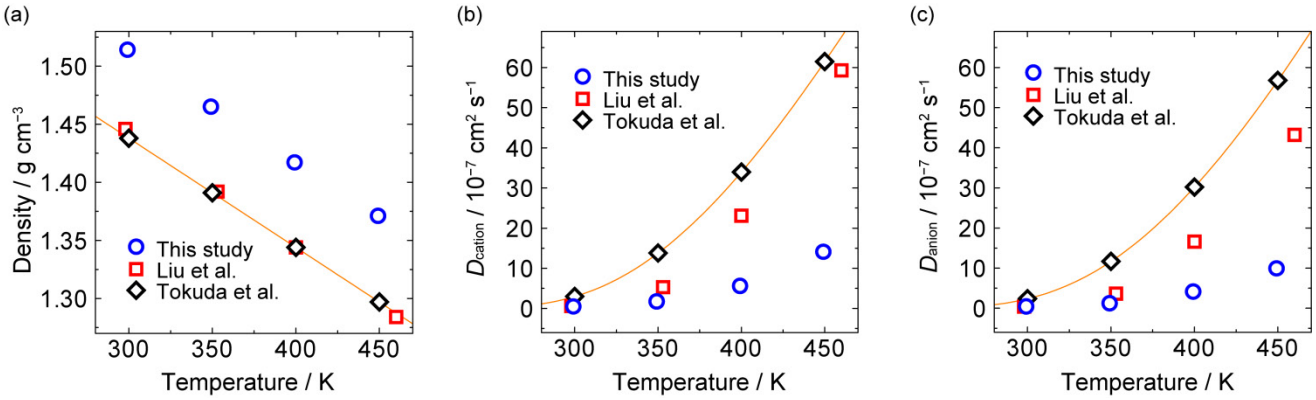

Fig. S1 Comparisons of computed and experimental (a) densities and self-diffusion coefficients of (b) BMIM cations and (c) TFSI anions. Computed values are from our simulations (circles) and from Ref. 42 by Liu et al. (rectangles) and experimental values are from Ref. 43 by Tokuda et al. (diamonds). Orange lines are guide for the eye.

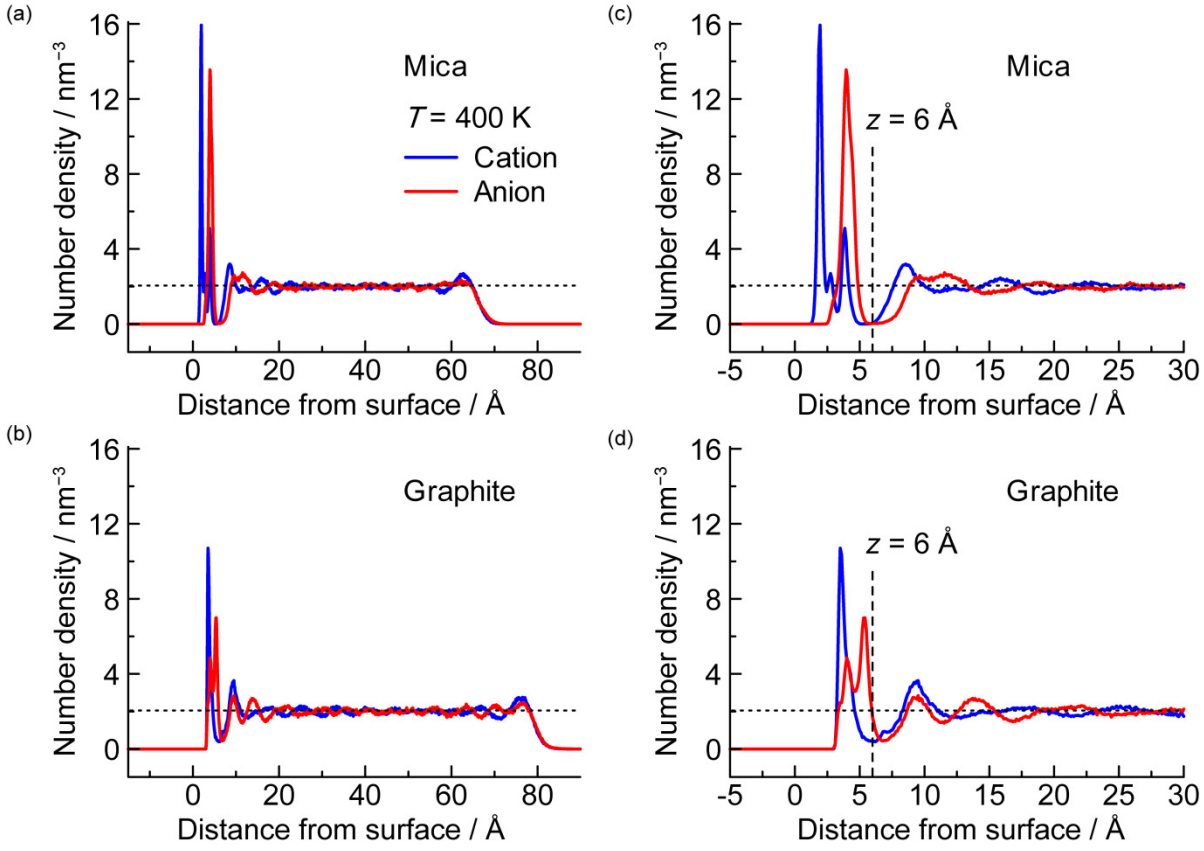

Fig. S2 (a)(b) Number density profiles of the cation and the anion at (a) mica and (b) graphite interfaces Horizontal dotted lines indicate the number density determined by the simulation of bulk BMIM-TFSI. (c)(d) Magnified number density profiles of (a) and (b), respectively. Vertical dashed lines define the first interface layer of BMIM-TFSI (z < 6 Å).

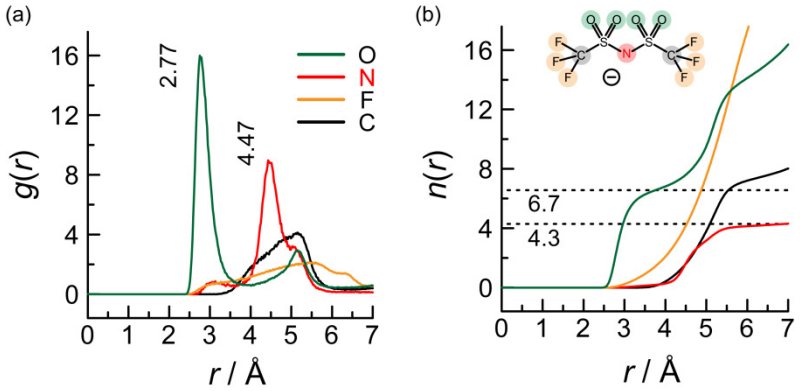

Fig. S3 (a) Partial radial distribution functions for K^+ cations and atoms of the TFSI anions calculated by MD simulation of 15 mol% K-TFSI dissolved in bulk BMIM-TFSI at 400 K. (b) Numbers of atoms of the TFSI anions coordinating to a K^+ cation within distance *r*.

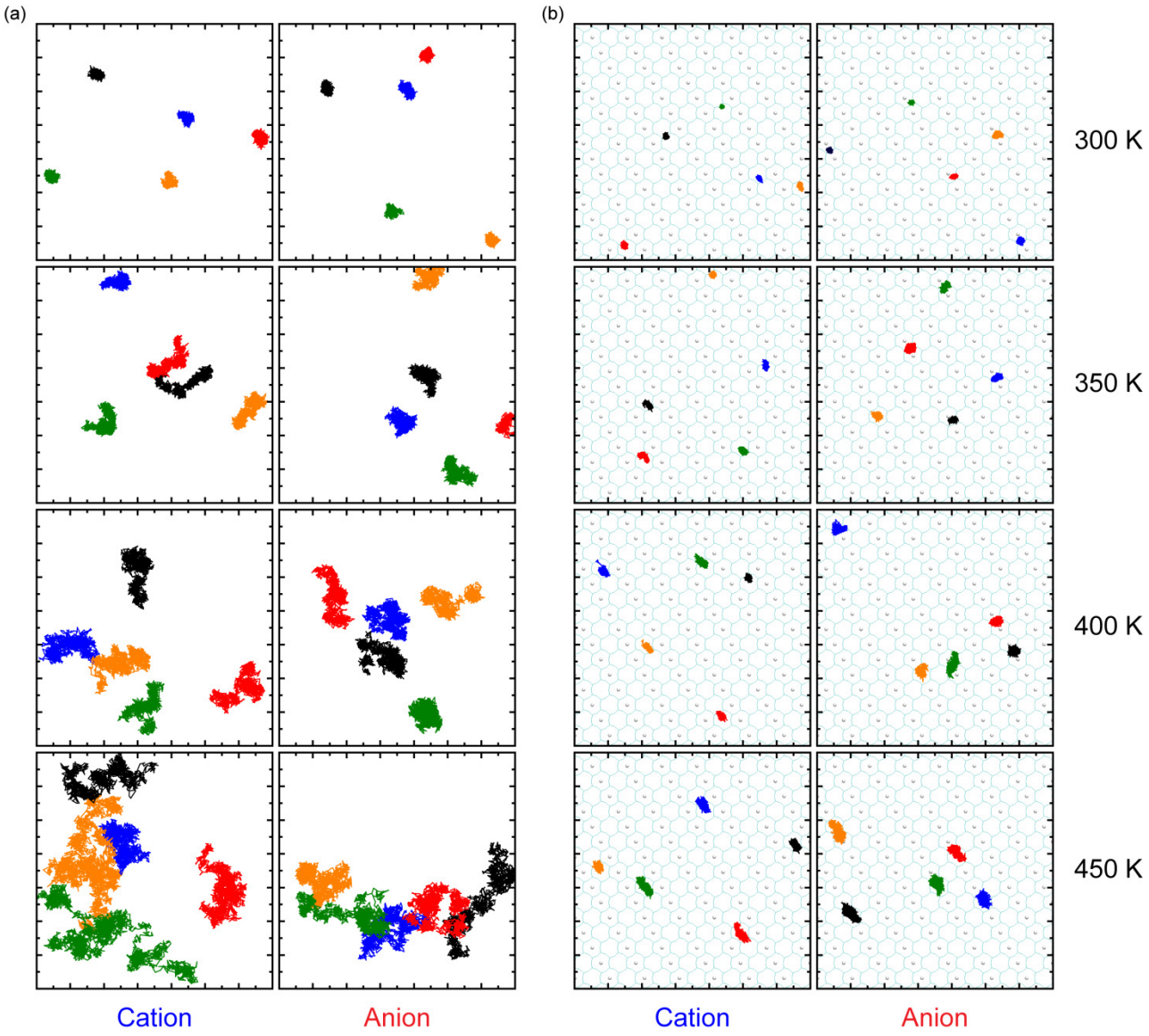

Fig. S4 The temperature dependences of XY contour maps (7×7 nm^2) for five BMIM cations and five TFSI anions during 5 ns simulation (a) at the bulk region (the initial z-positions were $33 < z < 35$ Å) and (b) at the first layer ($z < 6$ Å) of the mica interface. Different colors represent different ions. The substrate structures are superimposed in (b).

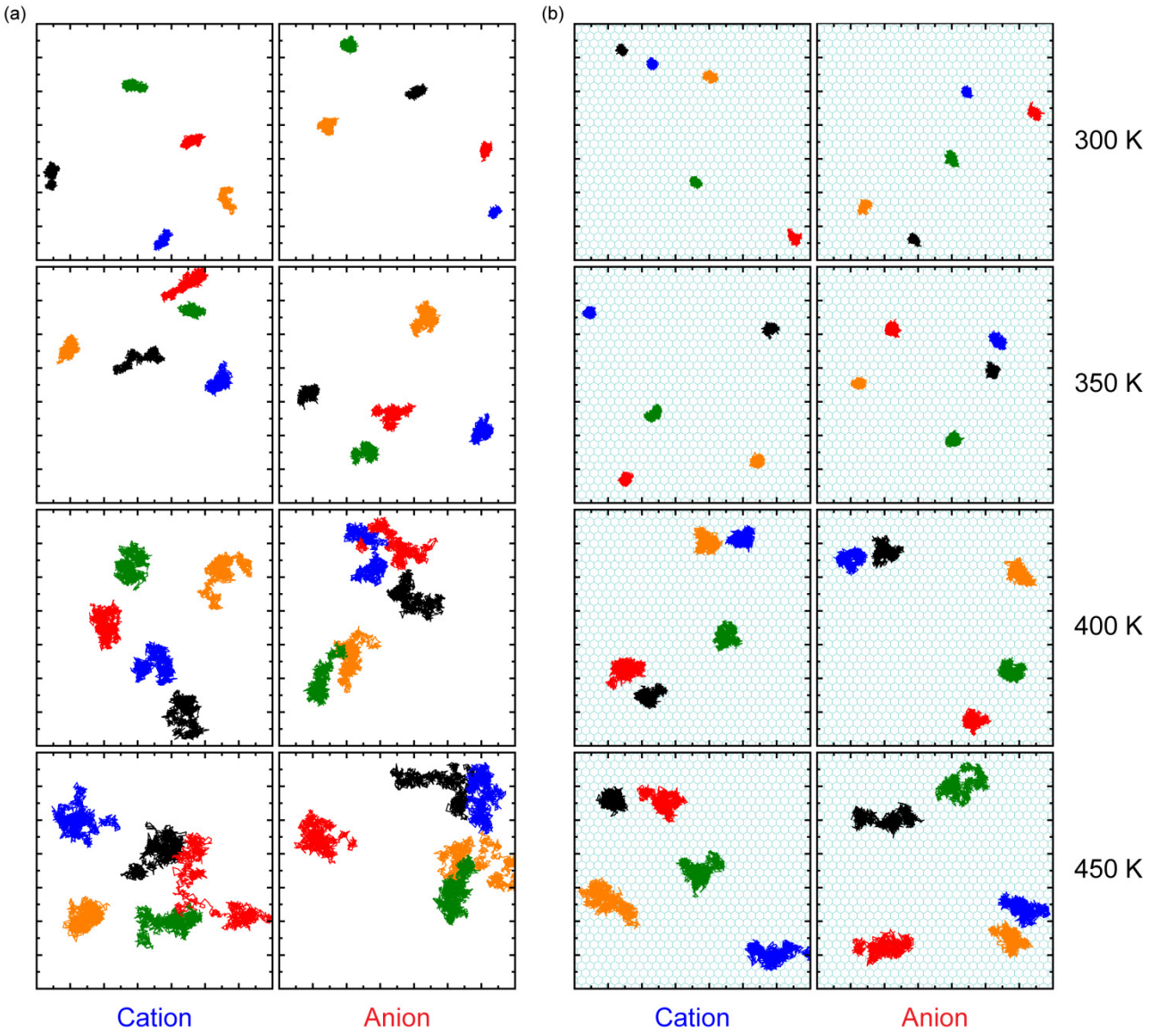

Fig. S5 The temperature dependences of XY contour maps (7×7 nm^2) for five BMIM cations and five TFSI anions during 5 ns simulation (a) at the bulk region (the initial *z*-positions were $40 < z < 43$ Å) and (b) at the first layer ($z < 6$ Å) of the graphite interface. Different colors represent different ions. The substrate structures are superimposed in (b).