Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Liquid/liquid interface layering of 1-butanol and [bmim]PF_6 ionic liquid: A nonlinear vibrational spectroscopy and molecular dynamics simulation study

Takashi Iwahashi,[a] Tatsuya Ishiyama,[b] Yasunari Sakai,[a] Akihiro Morita,[c,d] Doseok Kim[e] and Yukio Ouchi*[a]

[a]*Department of Organic and Polymeric Materials, Tokyo Institute of Technology, O-okayama, Meguro-ku, Tokyo, 152-8552, Japan.*

[b]*Department of Applied Chemistry, Graduate School of Science and Engineering, University of Toyama, Toyama 930-8555, Japan.*

[c]*Department of Chemistry, Graduate School of Science, Tohoku University, Aoba-ku, Sendai, 980-8578, Japan.*

[d]*Elements Strategy Initiative for Catalysts and Batteries (ESICB), Kyoto University, Kyoto 615-8520, Japan.*

[e]*Department of Physics, Sogang University, Seoul, 121-742, Republic of Korea.*

**To whom correspondence should be addressed. E-mail: ouchi.y.ab@m.titech.ac.jp Phone: +81-3-5734-2436. Fax: +81-3-5734-2876.*

Introduction

In this electronic supplementary information, the fitting parameters for all the SFG spectra discussed in the manuscript are given in the tables below.

Mode	Contact phase	Wavenumber / cm^{-1}	Peak Width / cm^{-1}	Amplitude, A_q	
				ssp	ppp
r^+ mode	Air	2883.4	7.0	23.5	8.4
	Butanol-d_9	2877.8	14.1	29.0	18.6
r^- mode	Air	2977.1	8.8	-1.5	42.5
	Butanol-d_9	2971.6	38.5	-17.7	79.2
d^+ mode	Air	2873.0	8.6	7.3	0.3
	Butanol-d_9	2857.9	10.0	7.7	3.5
d^- mode	Air	2925.1	12.1	8.4	10.9
	Butanol-d_9	2902.8	7.9	6.1	4.8
r^+_{FR} mode	Air	2948.0	7.8	21.8	10.5
	Butanol-d_9	2937.3	19.9	102.3	52.9

Table 1. Fitting parameters for SFG spectra taken within the CH stretch mode region of air/[bmim]PF_6 and butanol-d_9/[bmim]PF_6 interfaces shown in Fig. 4 of the manuscript.

Mode	Contact phase	Wavenumber / cm^{-1}	Peak Width / cm^{-1}	Amplitude, A_q	
				ssp	ppp
r^+ mode	Air	2074.1	10.6	22.0	1.5
	[bmim]PF_6	N/D	N/D	N/D	N/D
r^- mode	Air	2221.4	7.6	3.0	19.0
	[bmim]PF_6	2222.3	12.2	25.1	26.6

Table 2. Fitting parameters for SFG spectra taken within the CD stretch mode region of air/butanol-d_9 and butanol-d_9/[bmim]PF_6 interfaces shown in Fig. 5 of the manuscript. The amplitudes of r^+ mode at the butanol-d_9/[bmim]PF_6 interface could not be obtained because of the low SF signal weaker than the S/N level of the set-up.