

Supporting Information

Highly efficient sulfur dioxide capture by glyme-lithium salt ionic liquids

Shaoyang Sun,^a Yanxia Niu,^{a, b} Qiang Xu,^a Zuchen Sun,^a and Xionghui Wei^{*a}

^a Department of Applied Chemistry, College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

^b College of Chemistry and Chemical Engineering, Taiyuan University of Technology, Taiyuan 030024, China.

*Corresponding authors: Tel/Fax: +86-010-62670662. E-mail: xhwei@pku.edu.cn (X. H. Wei)

| Page No. | Contents |
|----------|---|
| S – 2 | Experimental Section. |
| S – 4 | Fig. S1 ¹ H-NMR spectra of tetraglyme, [Li-tetraglyme][NTf ₂] and [Li-tetraglyme][NTf ₂] after SO ₂ absorption, with D ₂ O as an external reference. |
| S – 5 | Fig. S2 SO ₂ absorption capacities of glyme-LiNTf ₂ ionic liquids at different temperatures with the pressure of SO ₂ equal to 1bar. |
| S – 6 | Fig. S3 SO ₂ absorption capacities of glyme-LiNTf ₂ ionic liquids at different SO ₂ partial pressures. |
| S – 7 | Fig. S4 SO ₂ absorption capacities of glyme-LiNTf ₂ ionic liquids in six absorption-desorption cycles. |
| S – 8 | Fig. S5 IR spectra of triglyme, [Li-triglyme][NTf ₂] and [Li-triglyme][NTf ₂] after SO ₂ absorption. |
| S – 9 | Fig. S6 SO ₂ absorption curves of different glyme-LiNTf ₂ ionic liquids at 293 K. |

1 Experimental Section

1.1 Materials

Glyme (G1), diglyme (G2), tetraethylene glycol and urea were purchased from Sinopharm Chemical Reagent Co. Ltd, while triglyme, tetraglyme, LiNTf₂, LiBF₄, LiOTf₂ and LiClO₄ were from J&K Chemical Ltd. All reagents were obtained in the highest purity grade possible, and directly used as received without further purification. Chromatographic grade Ethanol and distilled water were also used in this work. A certified standard pure SO₂ gas (>99.9 %), supplied by Beijing Gas Centre, Peking University (China), were employed to determine the SO₂ absorption capacity of ionic liquids.

1.2 Preparation of glyme-Li salt ionic liquids

All ionic liquids were prepared by simply mixing the lithium salts and glymes with stirring and heating. For example, the [Li-tetraglyme][NTf₂] was prepared by mixing the equimolar LiNTf₂ and tetraglyme, and then stirring at 353 K for half an hour. The formed liquids were purified by heating at 333 K in vacuum for 2 hours. No impurities were found in NMR and IR spectra.

1.3 Absorption and desorption of SO₂

The SO₂ absorption and desorption experiments were performed in an absorption tube with an inner diameter of 15 mm, which is in consistence with method in literature.¹ SO₂ gas of atmospheric pressure was bubbled through the samples (about 3 mL) in the absorption tube with a flow of 250 mL/min. The absorption tube was immersed in a circulating water bath to keep a certain temperature in absorption experiments, while an oil bath was used in desorption experiments. The absorption capacity of SO₂ was determined by an analytical balance (Sartorius BS 224S, with an uncertainty of 0.1 mg) at regular intervals. The uncertainty of absorption capacity is 0.01 mol SO₂/ mol IL. During the absorption experiments with different pressures, SO₂ was diluted by N₂ to obtain a mixed gas with a certain SO₂ partial pressure, by controlling the flow of SO₂ and N₂. The desorption experiments were conducted at 353 K with a N₂ flow of 200 mL/min, with the similar method mentioned above.

1.4 Spectral Measurements

IR and $^1\text{H-NMR}$ were employed to confirm the structure of ILs and investigate the interaction between ILs and SO_2 . The IR spectra were recorded on a Bruker Vector 22 FT-IR spectrophotometer, in which a typical thin film method was performed at ambient condition, with the wavenumber ranging from 400 cm^{-1} to 4000 cm^{-1} and a resolution of 1 cm^{-1} . A 500 MHz Bruker Avance III spectrometer was used to conduct the $^1\text{H-NMR}$ experiments. The NMR experiments were performed with external references. For external references, the samples and deuterated reagents were injected into capillary tubes ($25\text{ cm} \times 0.9\text{ mm}$) and NMR tubes ($17.8\text{ cm} \times 5\text{ mm}$), respectively. Then the capillary tube was inserted into the NMR tube to separate the samples from the solvents (deuterated reagents).

Reference

1. C. Wang, Y. Guo, X. Zhu, G. Cui, H. Li and S. Dai, *Chem. Commun.*, 2012, **48**, 6526-6528.

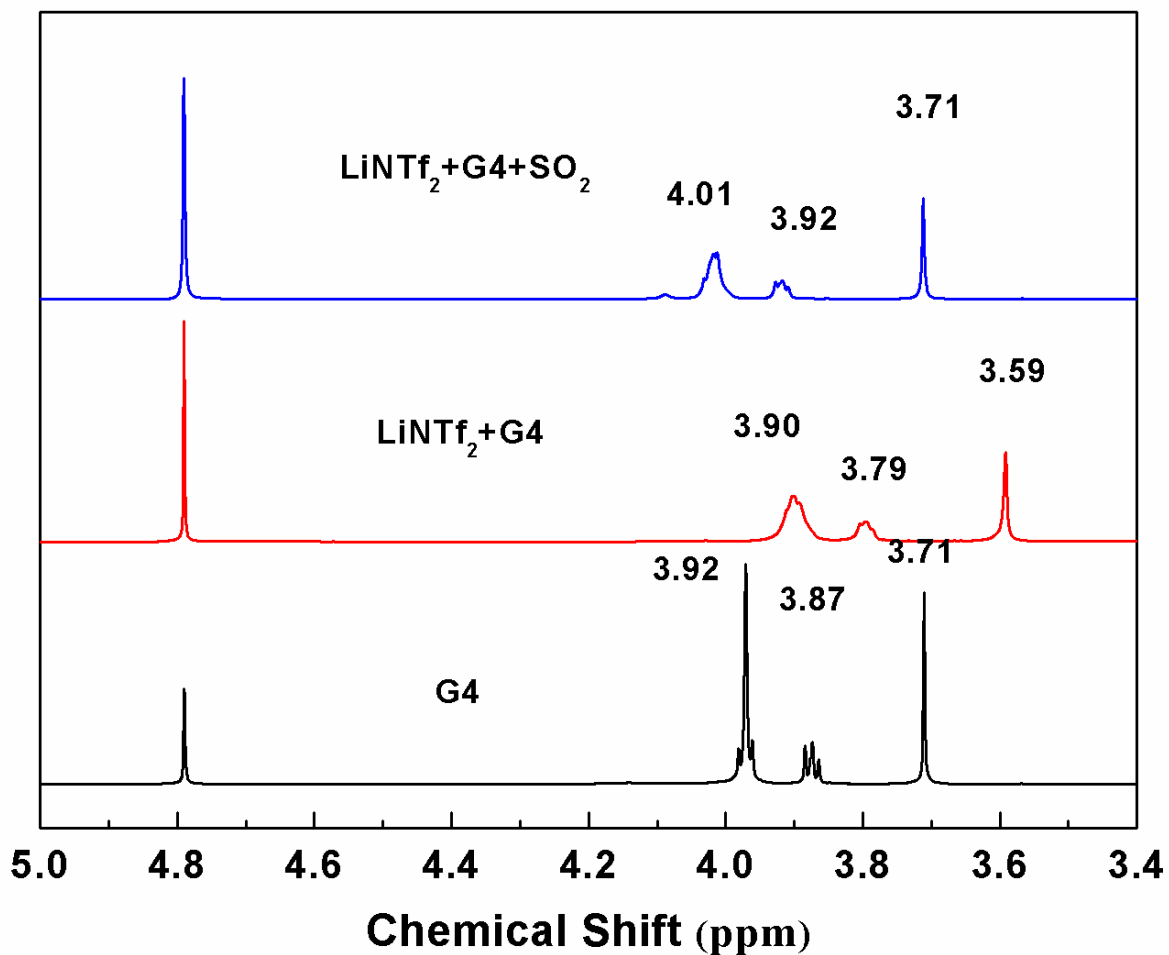


Fig. S1 $^1\text{H-NMR}$ spectra of tetraglyme, $[\text{Li-tetraglyme}][\text{NTf}_2]$ and $[\text{Li-tetraglyme}][\text{NTf}_2]$ after SO_2 absorption, with D_2O as an external reference

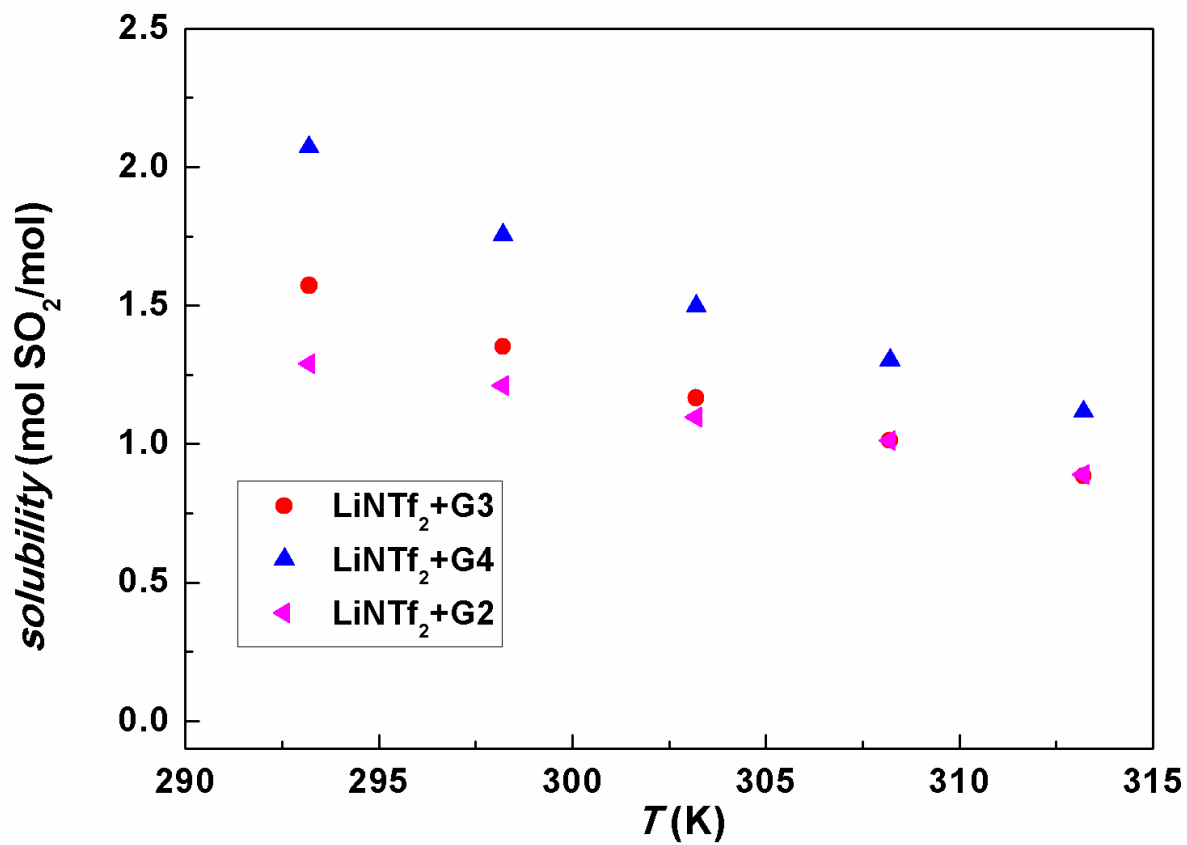


Fig. S2 SO₂ absorption capacities of glyme-LiNTf₂ ionic liquids at different temperatures with the pressure of SO₂ equal to 1bar.

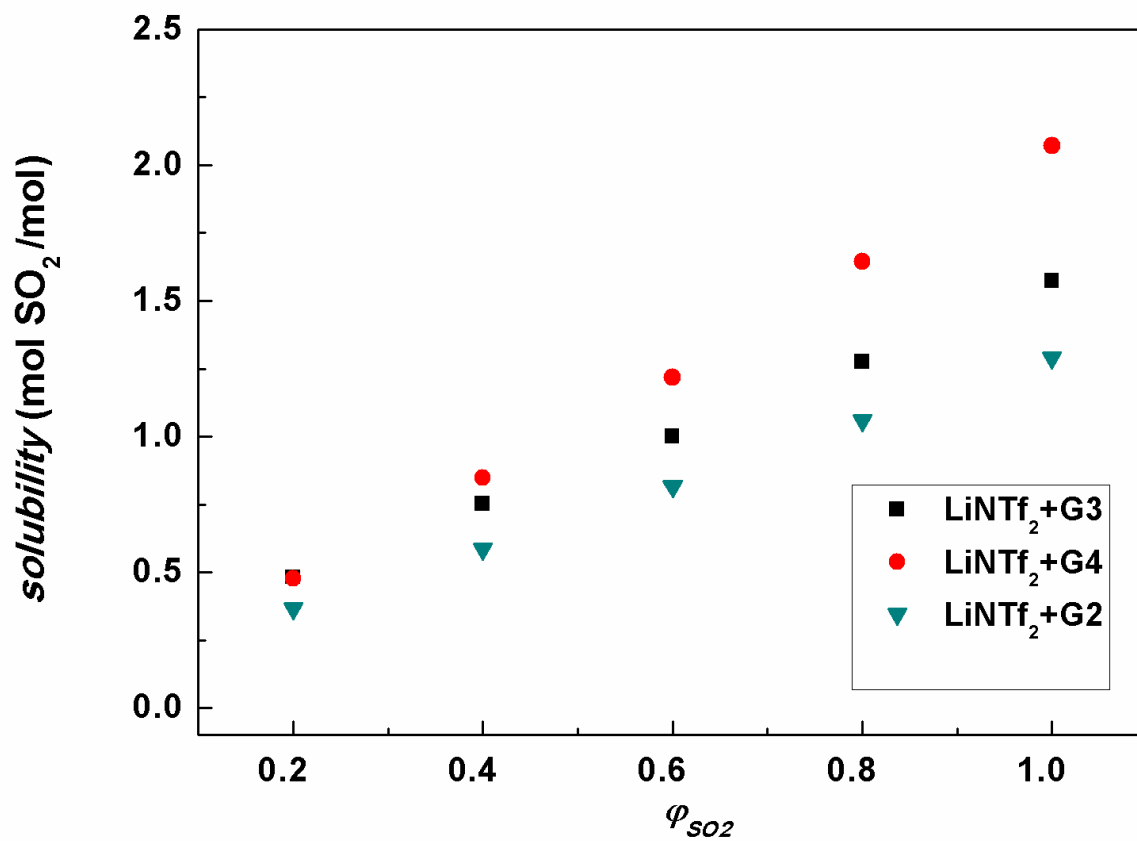


Fig. S3 SO₂ absorption capacities of glyme-LiNTf₂ ionic liquids at different SO₂ partial pressures.

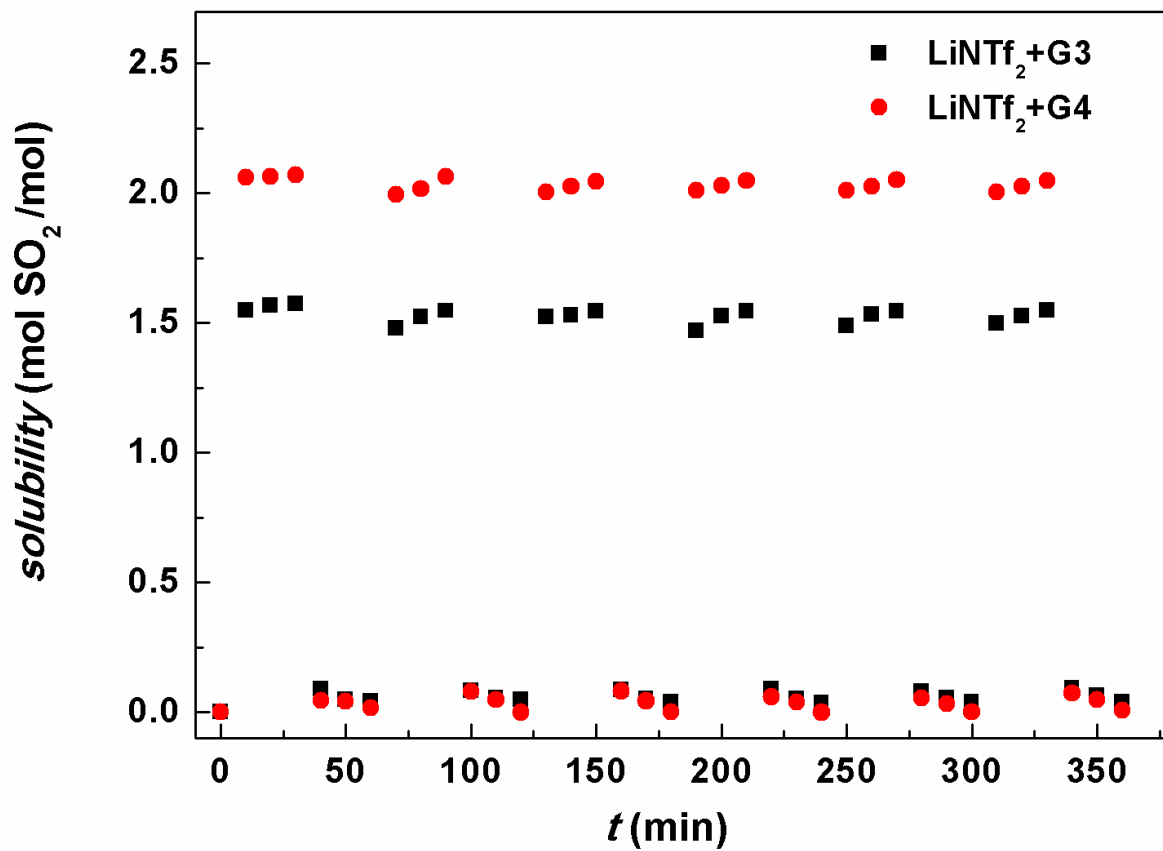


Fig. S4 SO₂ absorption capacities of glyme-LiNTf₂ ionic liquids in six absorption-desorption cycles.

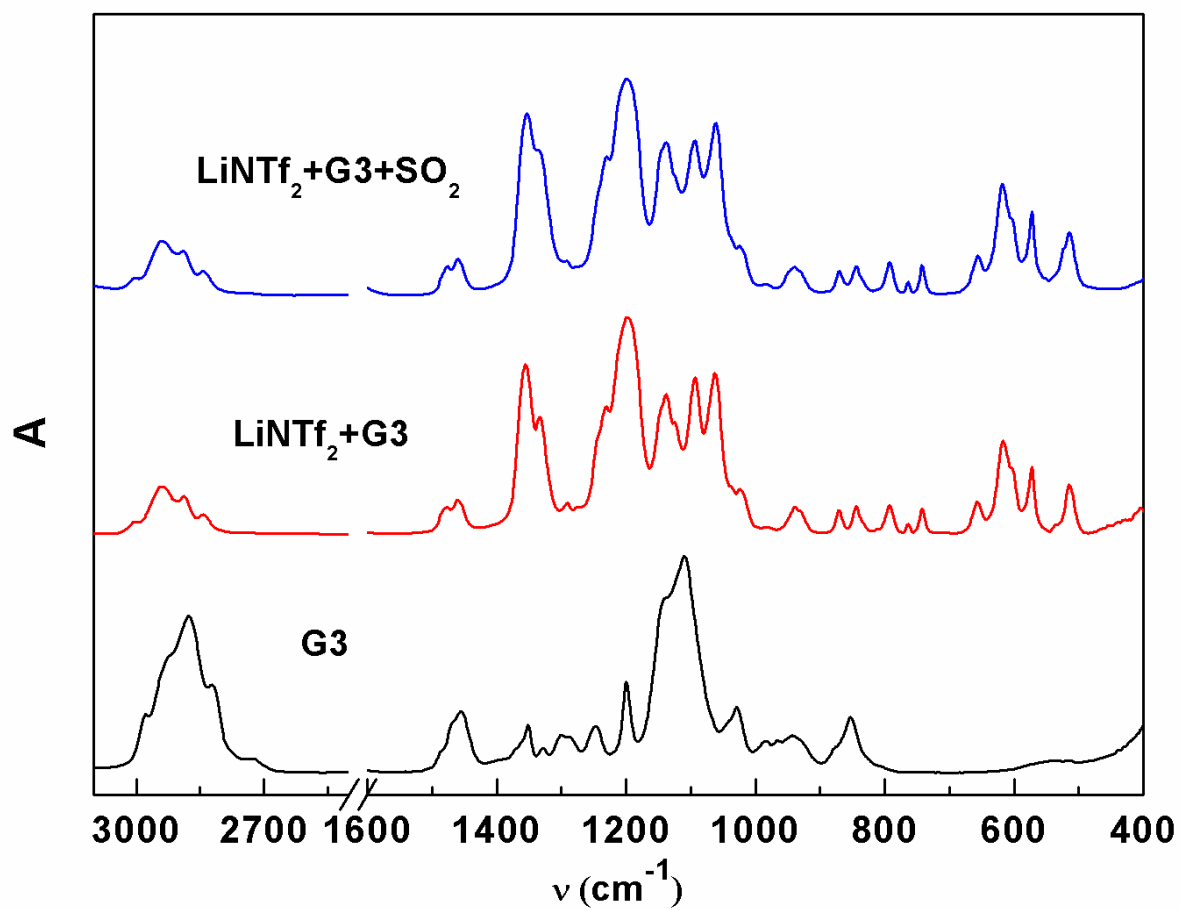


Fig. S5 IR spectra of triglyme, [Li-triglyme][NTf₂] and [Li-triglyme][NTf₂] after SO₂ absorption.

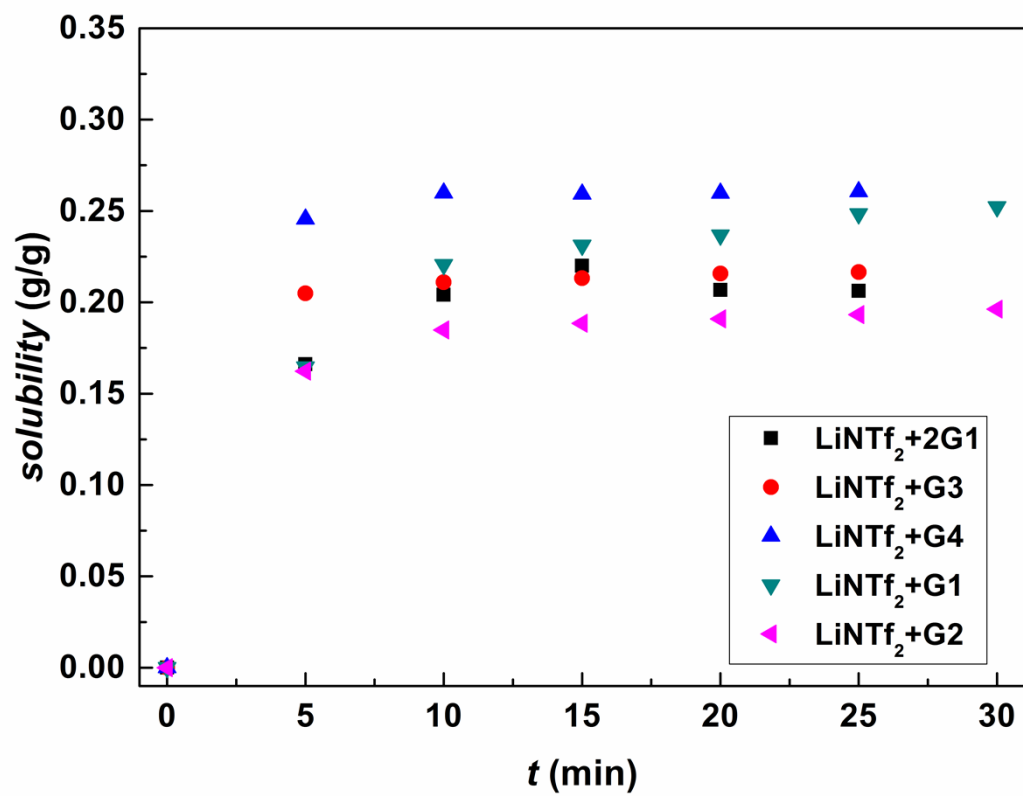


Fig. S6 SO₂ absorption curves of different glyme-LiNTf₂ ionic liquids at 293 K.