Supporting information

Supported ionic liquid phase (SILP) materials for removal of hazardous gas compounds – efficient and irreversible NH_3 adsorption.

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SILP preparation

Usually, between 15 and 30 g of SILP material has been prepared. For the benchmark test regarding broadband capability, the mass of prepared $[C_2C_1Im]Cl\text{-}CuCl_2$ SILP material amounted to 117 g. In order to distribute the ionic liquid more evenly across the inner surface of the spherical carbon, the wet impregnation method was enhanced by an ultrasonication step applying a UP200S ultrasonic sonotrode from Hielscher. The sonotrode was placed in an oil bath outside the flask containing the impregnation suspension. The amplitude of ultrasonic waves was set to 50% with an interval of 0.5 s. With a rotary evaporator, the solvent was removed. The SILP material was further dried at 120°C and 0.01 mbar vacuum for 18 h. With this impregnation method, the ionic liquid was always fully deposited within the spherical carbon resulting in a dry and pourable material with no visible ionic liquid.

Solubility measurements

The ionic liquids were placed in the pressure chamber 3 and the lid was closed. The chamber 3, the reservoir 2 and the transfer lines were evacuated for 1 h under elevated temperature. Afterwards the valves between the two chambers were closed and the required temperature was adjusted.

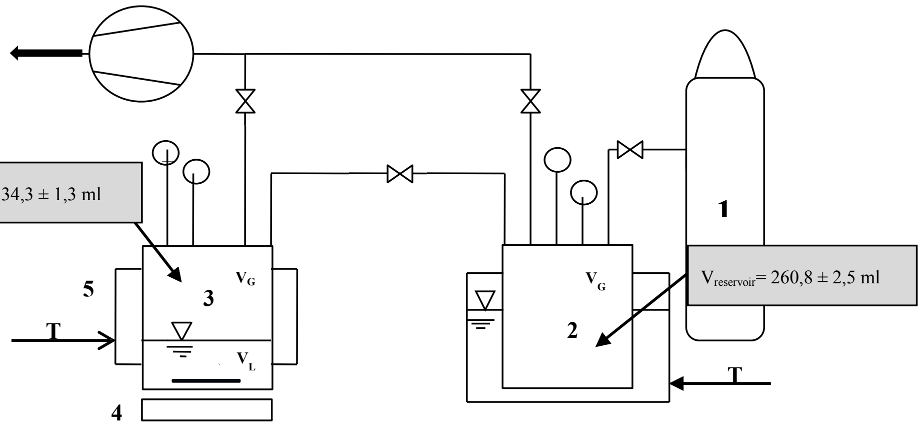

Figure S1. *Schematic view of the experimental set up used for gas solubility measurements of ammonia. 1 gas supply, 2 gas reservoir, 3 pressure chamber, 4 magnetic stirrer, 5 heating.*

Ammonia gas was dosed into chamber 2 and equilibration was awaited for at least 30 min. The pressure inside the chambers as recorded and the transmission line valve was opened, allowing ammonia to enter the pressure chamber. The pressure loss of chamber 2 was monitored online via a pressure transducer.

Complexation of ammonia

Figure S2 illustrates the color change of the investigated ionic liquids within the gas solubility measurements.

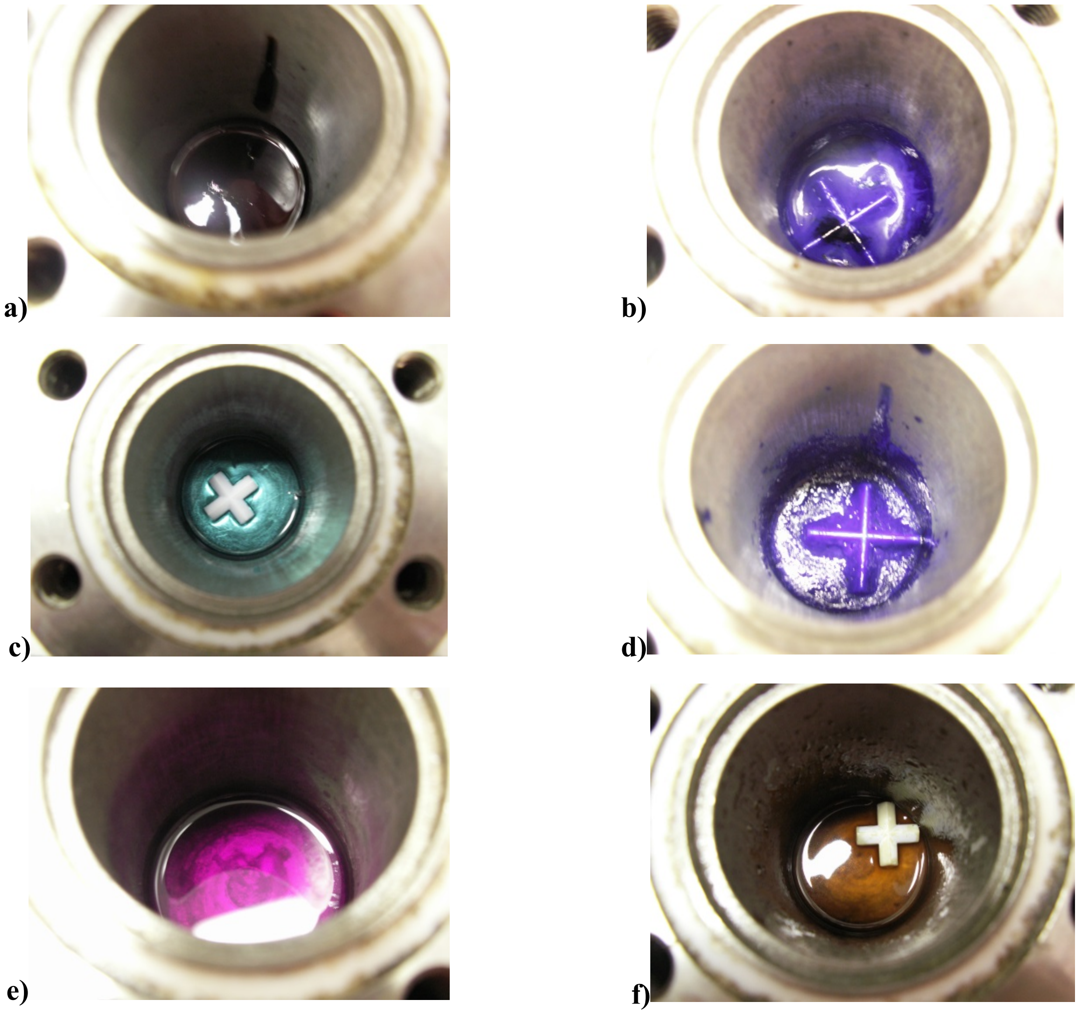

Figure S2. *Colour change of ILs observed within the gas solubility measurements of ammonia. a) $[C_8C_1Im]Cl/CuCl_2$ (X_{CuCl2} = 0.5) before ammonia absorption. b) $[C_8C_1Im]Cl/CuCl_2$ (X_{CuCl2} = 0.5) after ammonia absorption. c)$[C_8C_1Im][NTf_2]/Cu(NTf_2)_2$ ($X_{Cu(NTf2)2}$ = 0.05) before ammonia absorption. d) $[C_8C_1Im][NTf_2]/Cu(NTf_2)_2$ ($X_{Cu(NTf2)2}$ = 0.05) after ammonia absorption. e) $[C_8C_1Im][NTf_2]/Co(NTf_2)_2$ ($X_{Co(NTf2)2}$ = 0.15) before ammonia absorption. f) $[C_8C_1Im][NTf_2]/Co(NTf_2)_2$ ($X_{Co(NTf2)2}$ = 0.15) after ammonia absorption.*

Mathematical fitting of breakthrough curves

All breakthrough curves were fitted using an empirical formula of a hyperbolic tangent function as shown in Equation (S1).

$$y(t) = a \cdot \tanh(b \cdot t + c) + a \tag{S1}$$

In this time-dependent function of the normalized ammonia concentration, the parameter *a* represents the normalized concentration regime and ideally has a value of 0.5, meaning that the normalized concentration starts at 0 and has a maximum value of 1. Due to the calculation with mean values during calibration of the gas chromatographic detector and a resulting systematic error, a deviation from the maximum ammonia concentration can occur. In case the initial fit of the data does not result in a value of 0.5, the deviation is accounted for by norming and fitting a data series with a factor of 0.5/*a*.

Variable *b* describes the effective absorption kinetics. This includes the mass transport of ammonia from the gas phase into the ionic liquid film resembled by pore diffusion and the physical solubility of ammonia in the ionic liquid. Additionally, the effective absorption kinetics takes account of the chemical reaction of dissolved ammonia into metal amine complexes. At the function's inflection point (in the region of c_{out}-c_{in}=0.5), the slope is the product of the parameters *a* and *b*. Thus, with a constant parameter *a=0.5*, the absorption rate is solely represented by variable *b*. A large value of *b* indicates a fast absorption of ammonia, but also a quicker saturation of the SILP material. Nevertheless, fast absorption kinetics designate a high performance SILP absorber of ammonia with minimized mass transport limitations. Also, it's evidence of an exact measurement of the break-through time, because flat curves can be caused by channeling of ammonia through a non-ideal bed of SILP material and can distort the break-through time.

Thermal stability

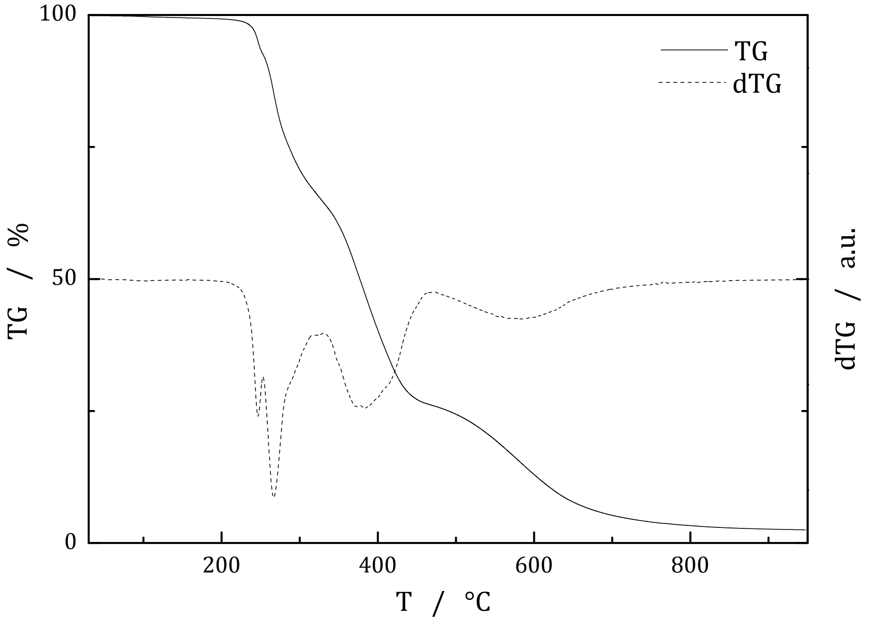

***Figure S3**: Thermo-gravimetric analysis of the ionic liquid melt [C_2C_1Im]Cl/$CuCl_2$ (x_{CuCl2} = 0.57) in the temperature range of 30-950°C (heating rate: 10 K min^{-1})*

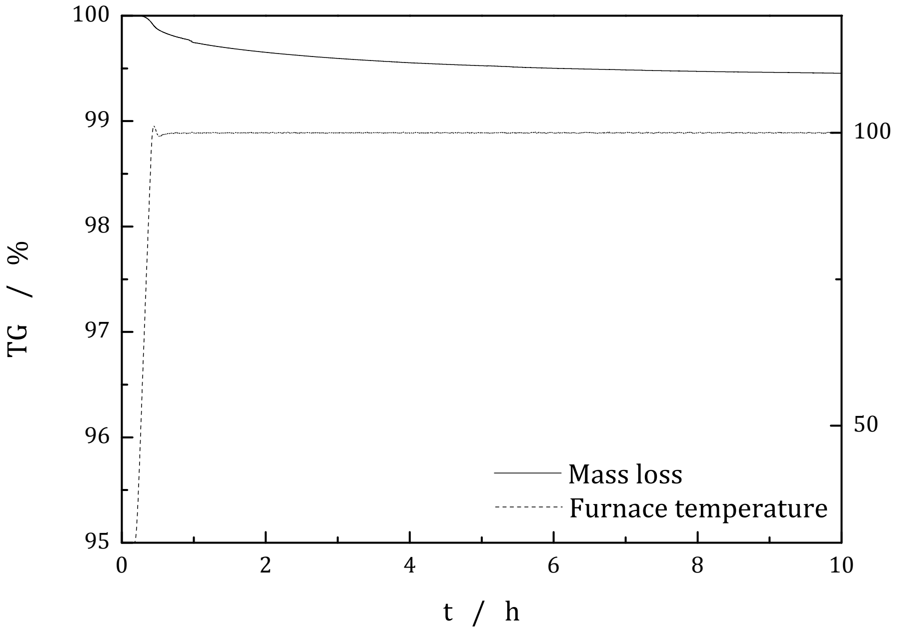

***Figure S4**: Thermo-gravimetric long-term analysis at 100°C for 10 h of SILP absorber material coated with [C_2C_1Im]Cl/$CuCl_2$ (x_{CuCl2} = 0.57) α_{IL} = 0.2*