Supporting information

Development and systematic evaluation of aqueous triazole chloride-based deep eutectic solvents for efficient CO2 capture

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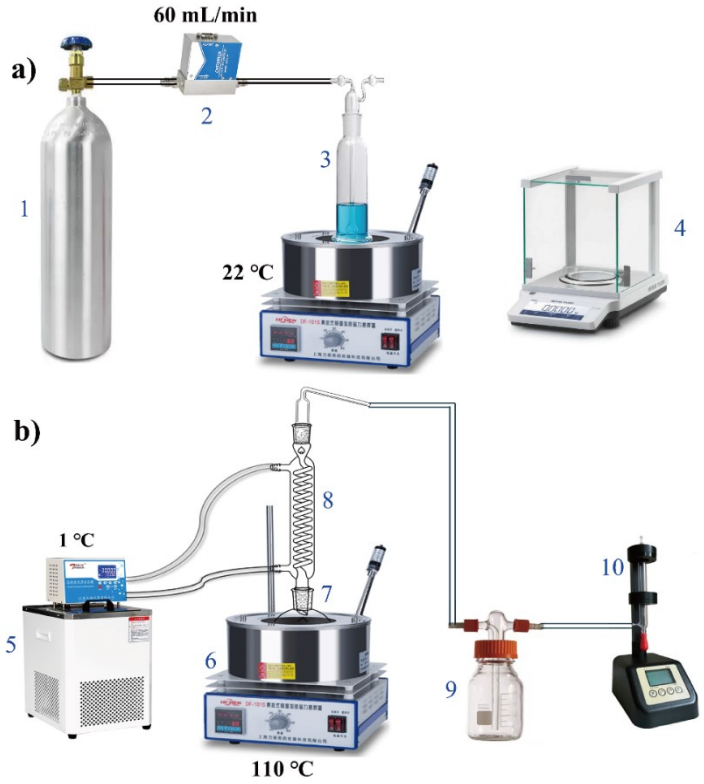

Fig. S1. Schematic diagram of the CO_2 a) absorption and b) desorption apparatus (1 - CO_2; 2 – mass flow controller; 3 - absorption bottle; 4 - electronic balance; 5 - low-temperature constant temperature bath; 6 - oil bath; 7 - round-bottom flask; 8 - serpentine condenser; 9 - sulfuric acid; 10 - electronic soap film flowmeter).

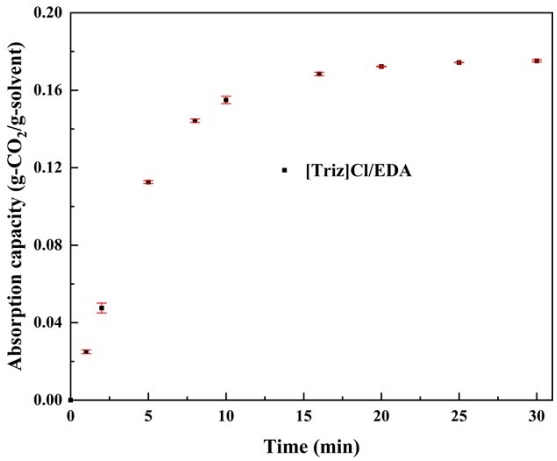

Fig. S2. Experimental results of CO_2 absorption capacity in 30 wt% [TrizCl][EDA] aqueous solutions.

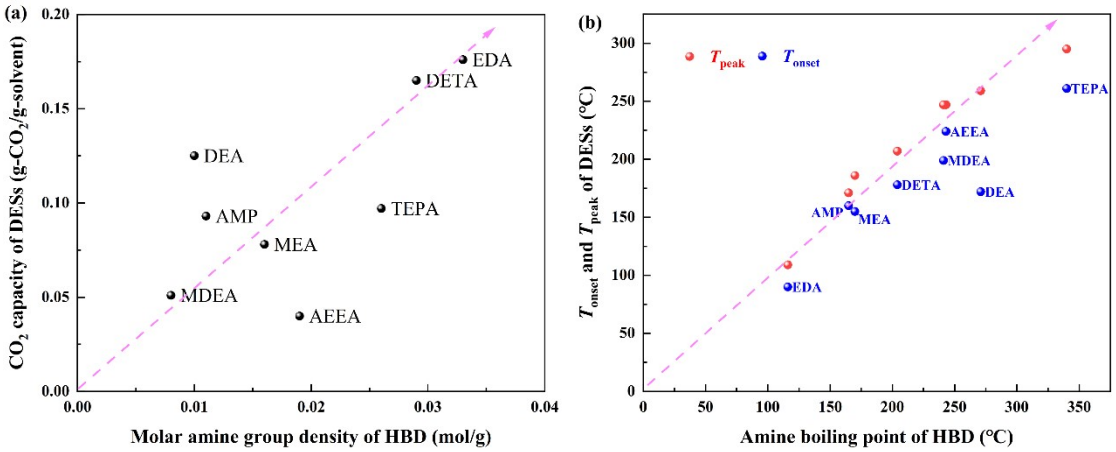

Fig. S3. Structure-property relationships of [Triz]Cl/amine.

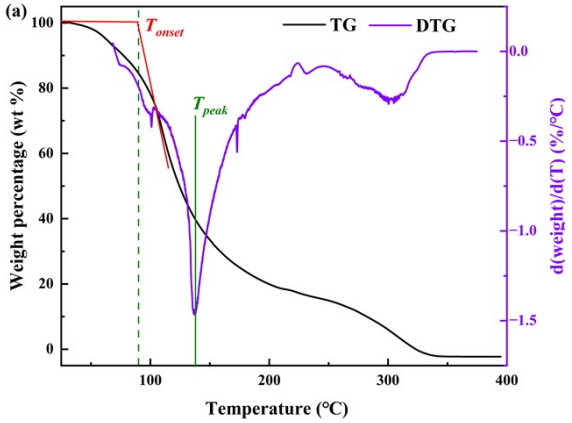

Fig. S4. TG and DTG curves of [TrizCl][EDA].

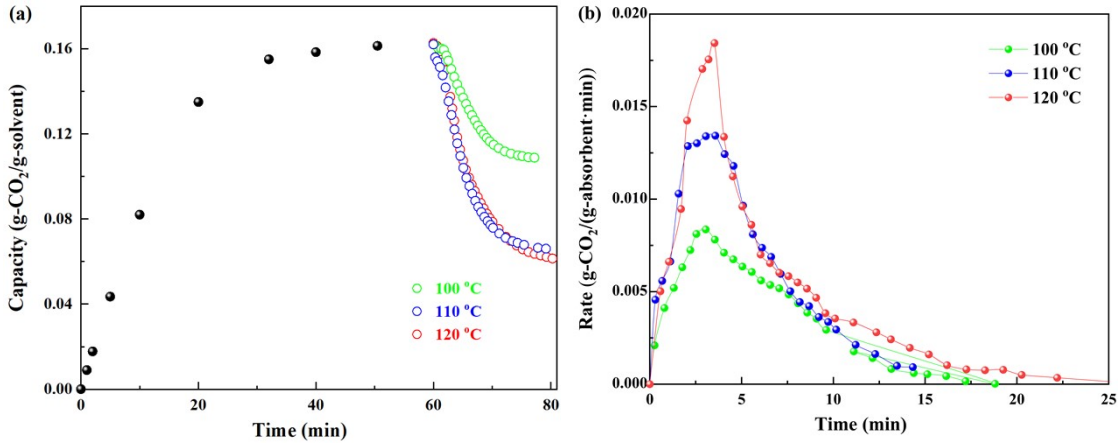

Fig. S5. (a) The variation of CO_2 capacity with time for 30 wt% MEA; and (b) the variation of the CO_2 desorption rate with time at different temperatures.

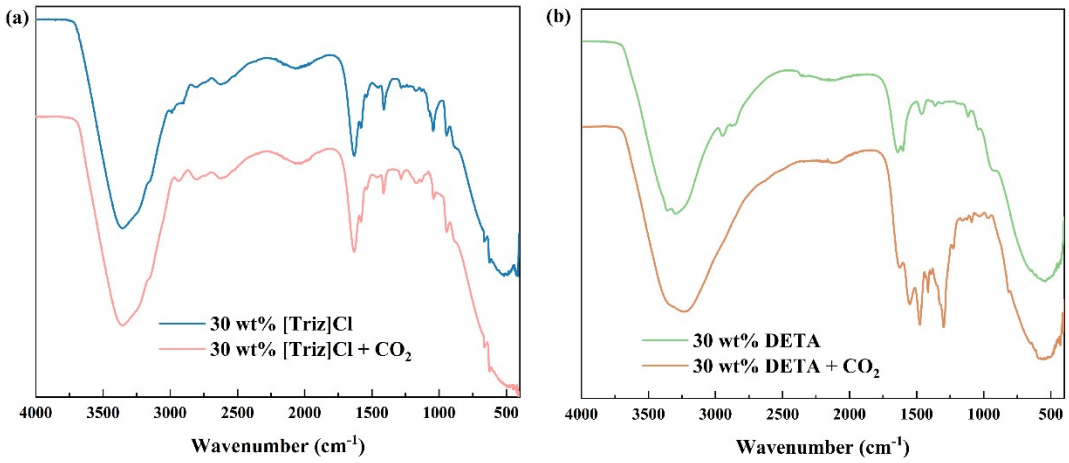

Fig. S6. FTIR of (a) 30 wt% [Triz]Cl and (b) 30 wt% DETA before and after CO_2 absorption.

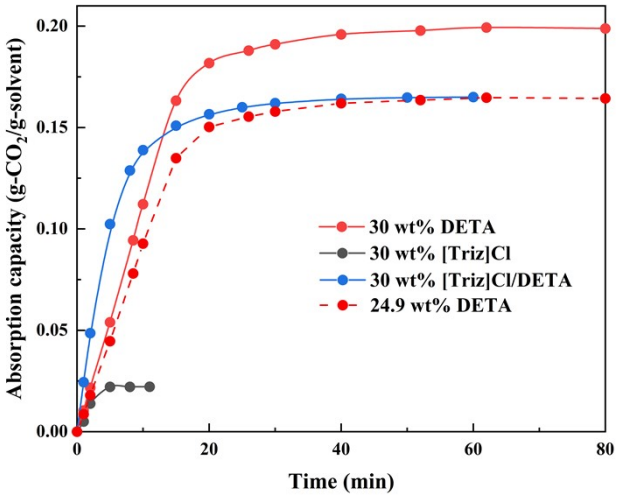

Fig. S7. CO_2 absorption of 30 wt% DETA, [Triz]Cl, [Triz]Cl/DETA, as well as that of 24.9 wt% DETA at 22 °C.

Section 2: Calculation methods

2.1 Normalization: Min-Max scaling methods

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}} \quad \text{(Eq. S1)}$$

2.2 Calculation procedure for simplified regeneration energy

2.2.1 Assumptions

(1) The regeneration energy is approximated by the sensible heat required to heat the solvent from the absorption temperature T_{abs} to the desorption temperature T_{des}.

(2) The 30 wt% aqueous [Triz]Cl/DETA solution is dominated by DETA and water; thus, its heat capacity is approximated by that of aqueous DETA solutions.

(3) The specific heat capacity of 30 wt% aqueous MEA has been reported to be in the range of 3.73-3.90 kJ·kg^{-1}·K^{-1} (*J. Chem. Eng. Data* 1997, 42, 5, 1004-1006; *Appl. Energ.* 2016, 168, 394-405). 30 wt% aqueous DETA solutions exhibit isobaric heat capacities in the range of 3.7-3.9 kJ·kg^{-1}·K^{-1}, reported by Lin et al. (*Thermochimica Acta* 2014, 575, 34-39).

2.2.2 Calculation of sensible regeneration energy

For a given solvent, the sensible heat required to raise the temperature from T_{abs} to T_{des} is estimated as:

$$Q_{sens} \approx c_p \cdot \Delta T$$

where Q_{sens} is the sensible heat (kJ·kg^{-1}·solvent), c_p is the specific heat capacity (kJ·kg^{-1}·K^{-1}), and $\Delta T = T_{des}$-T_{abs}.

To compare different solvents, Q_{sens} is normalised by the cyclic CO_2 loading n_c (g-CO_2/g-solvent), yielding an approximate sensible heat requirement per unit CO_2, E_{reg}^{sens}:

$$E_{reg}^{sens} \approx \frac{Q_{sens}}{n_c}$$

where E_{reg}^{sens} is expressed in $kJ \cdot kg^{-1} \cdot CO_2$.