

Supplementary Information for:

Impact of α -D-glucose pentaacetate on the selective separation of CO₂ and SO₂ in supported ionic-liquid membranes

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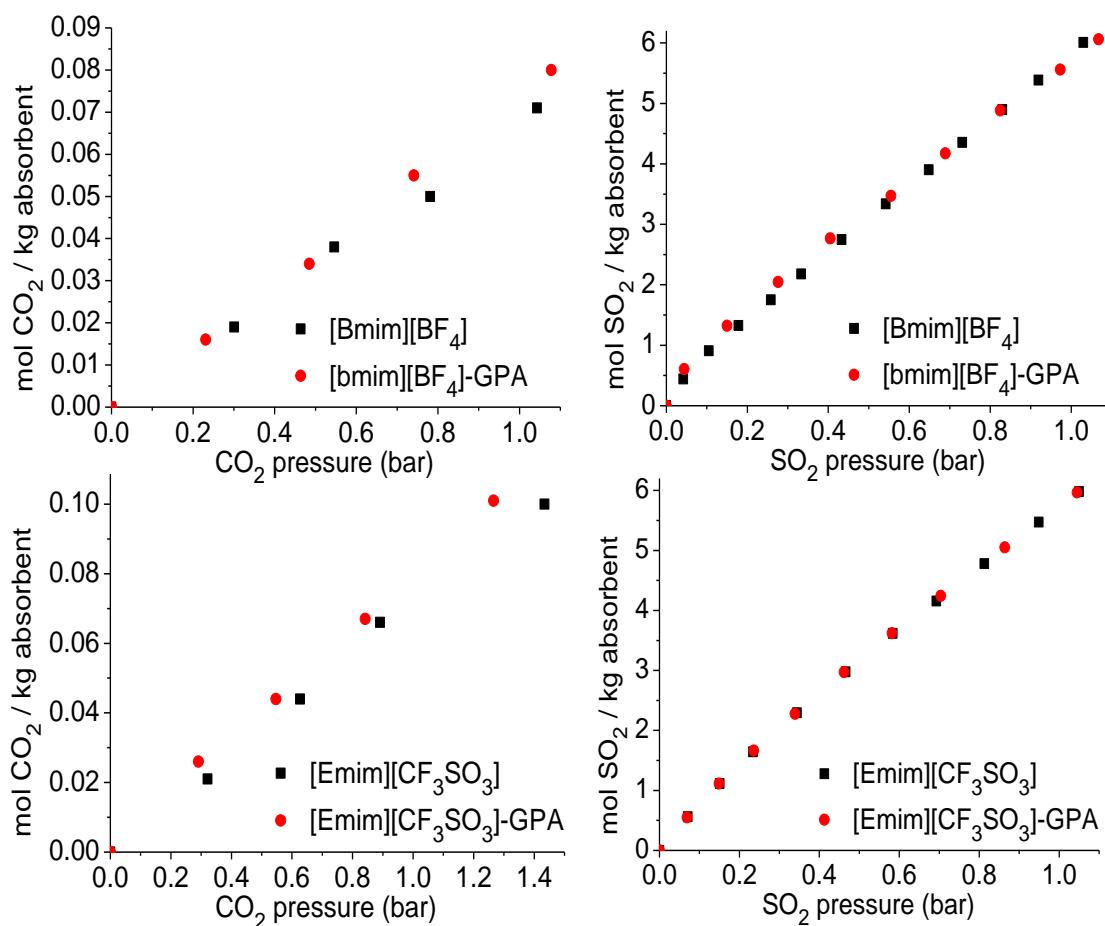


Fig. S1 The solubility of CO₂ and SO₂ in different absorbents.

Table S1. The dependence of gas solubility (Sol) in ILs on the pressure (P).^a

	CO ₂		SO ₂	
	Relationship	R ²	Relationship	R ²
[Bmim][BF ₄]	<i>Sol = 0.067P</i>	0.997	<i>Sol = 5.65P</i>	0.998
[Bmim][BF ₄]-GPA	<i>Sol = 0.075P</i>	0.999	<i>Sol = 5.43P</i>	0.994
[Emim][CF ₃ SO ₃]	<i>Sol = 0.071P</i>	0.998	<i>Sol = 5.59P</i>	0.997
[Emim][CF ₃ SO ₃]-GPA	<i>Sol = 0.079P</i>	0.999	<i>Sol = 5.63P</i>	0.996

^a Obtained by data regression analysis in Fig. S1. R² is the correlation coefficient.

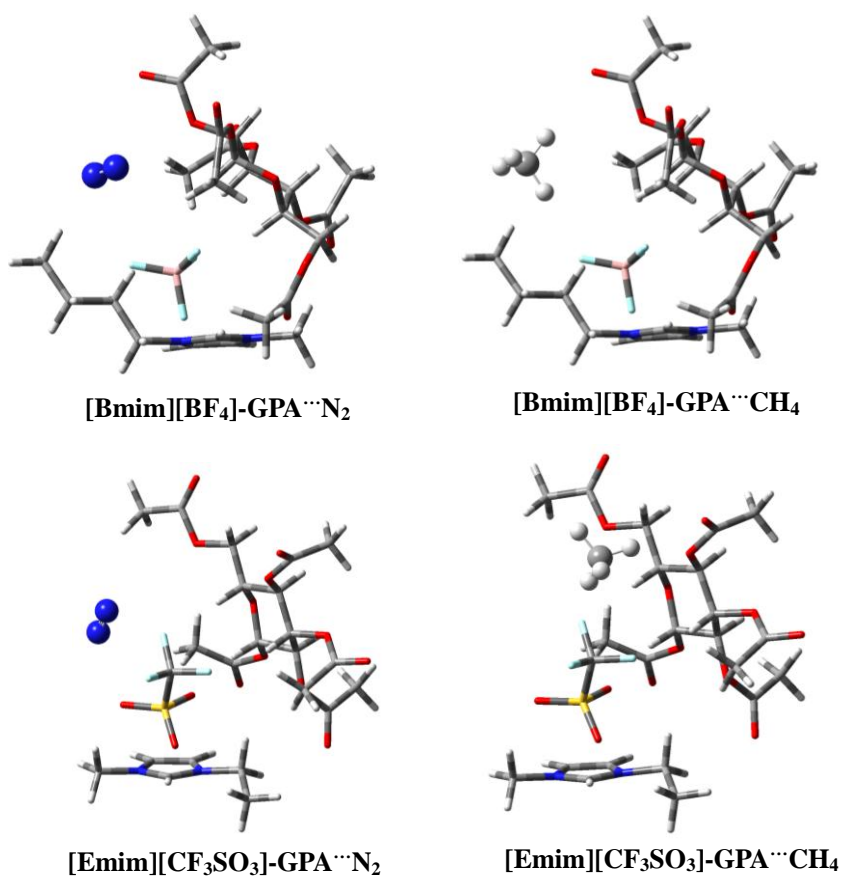


Figure S2. The optimized structures of IL-GPA...N₂ and IL-GPA...CH₄.

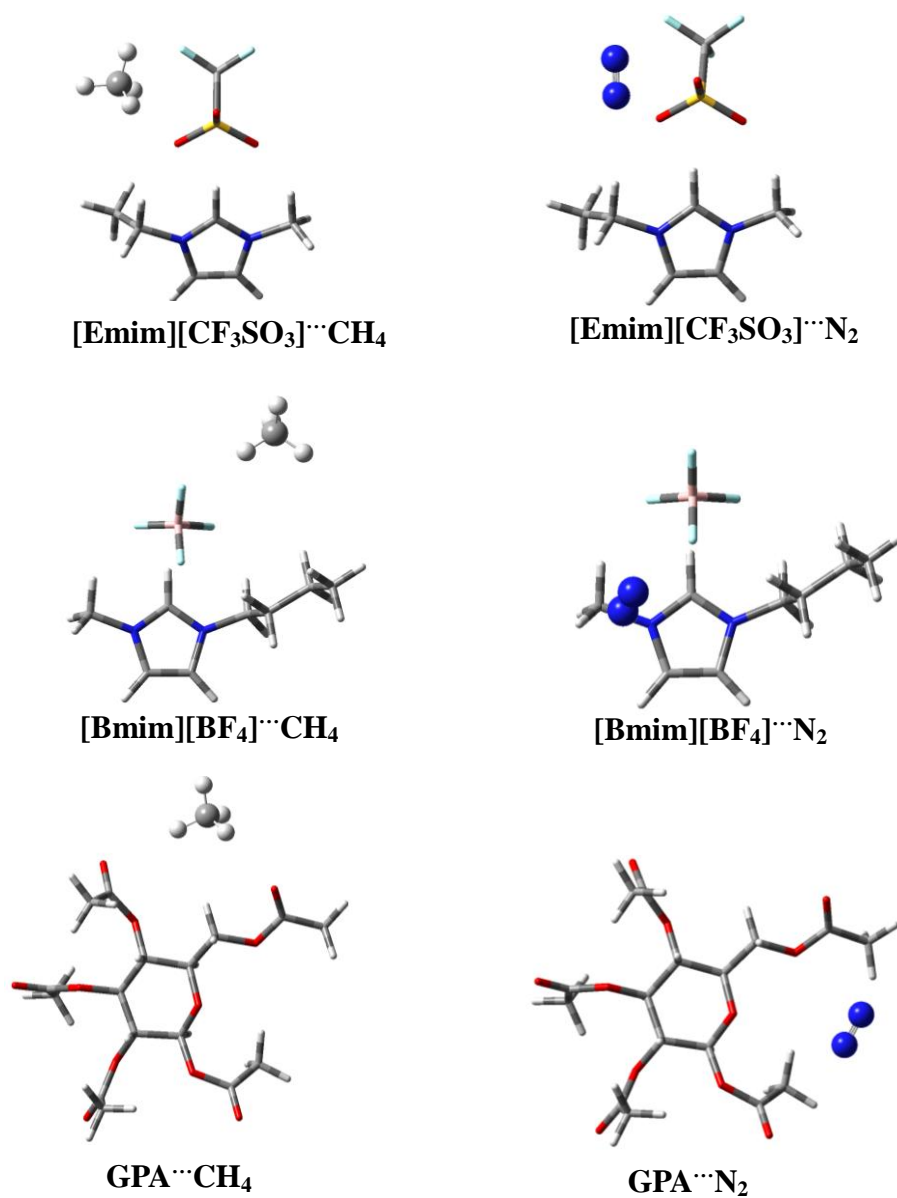


Figure S3. The optimized structures of IL⁺N₂, IL⁺CH₄, GPA⁺N₂, and GPA⁺CH₄.

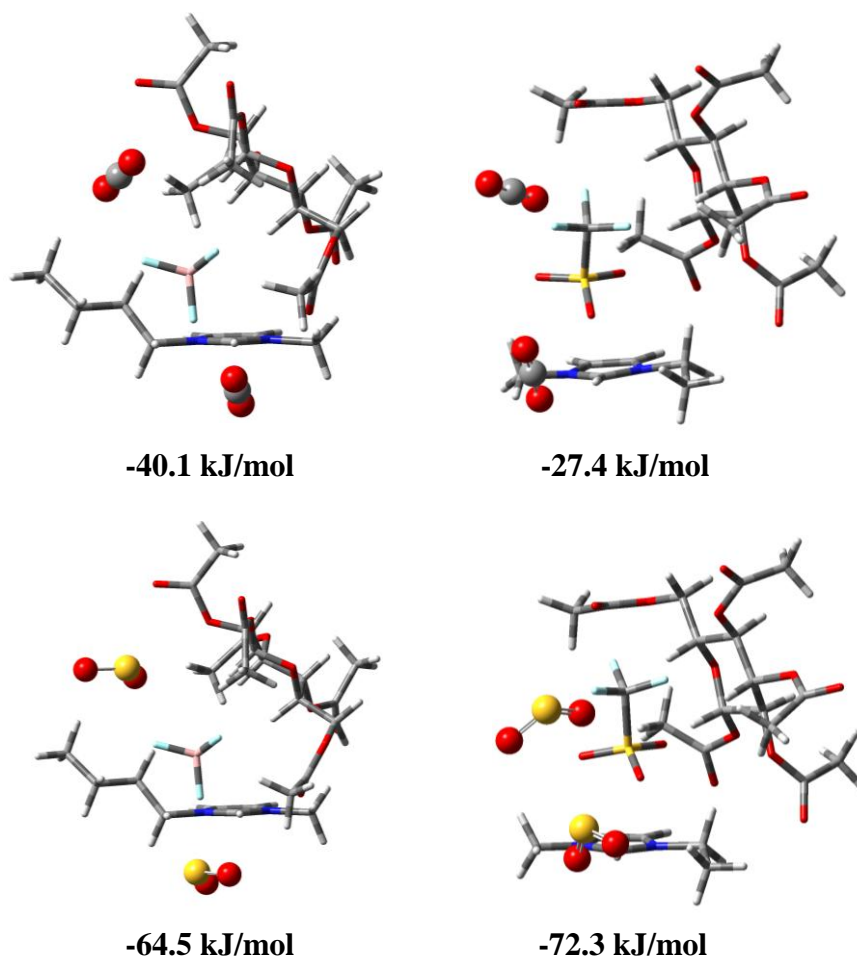


Figure S4. The optimized structures of IL-GPA \cdots CO₂, and IL-GPA \cdots SO₂. The shown values mean the binding energies between IL-GPA and CO₂/ SO₂.

Table S2. The 2-molecules interaction energies (in kJ/mol) of IL^{***}gas, GPA^{***}gas, or IL-GPA^{***}gas.

	2CO ₂	2SO ₂
[Bmim][BF ₄]	-33.7	-71.0
[Emim][CF ₃ SO ₃]	-27.3	-79.9
GPA	-19.2	-38.8
[Bmim][BF ₄]-GPA	-40.1	-64.5
[Emim][CF ₃ SO ₃]-GPA	-27.4	-72.3

^a The structures of two gas molecules interaction were presented in [Fig. S2~S5](#) of Supplementary Information.

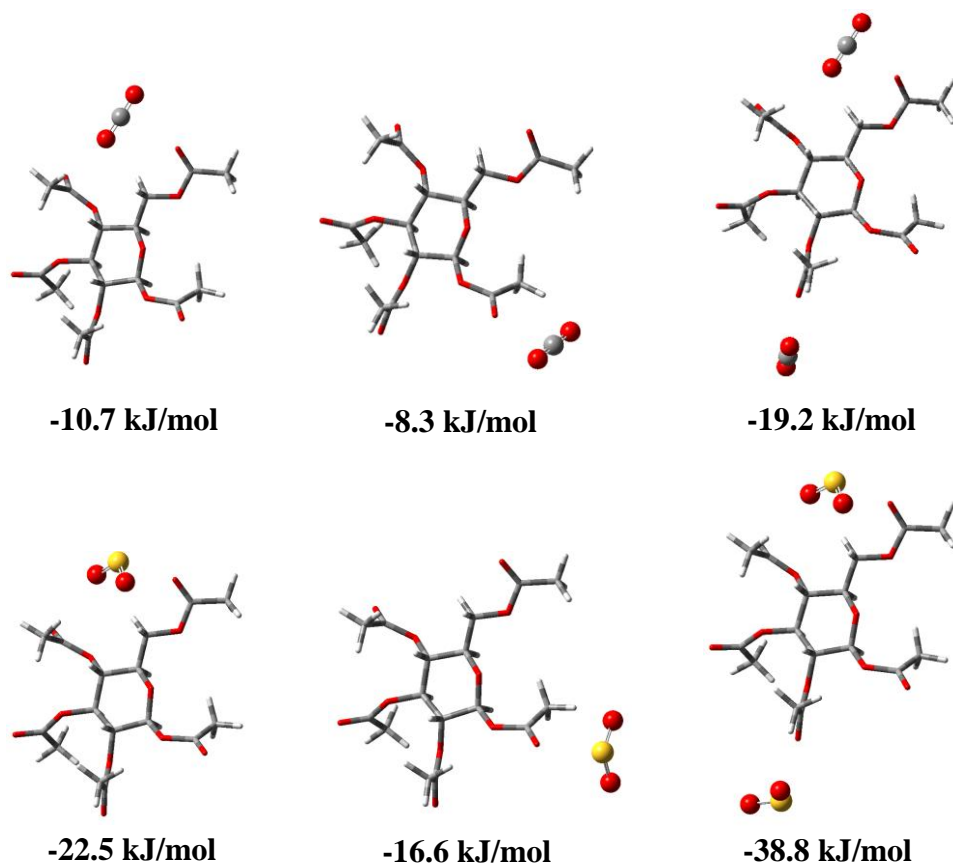


Figure S5. The optimized structures of GPA \cdots CO₂ and GPA \cdots SO₂. The shown values mean the binding energies between GPA and CO₂/SO₂.

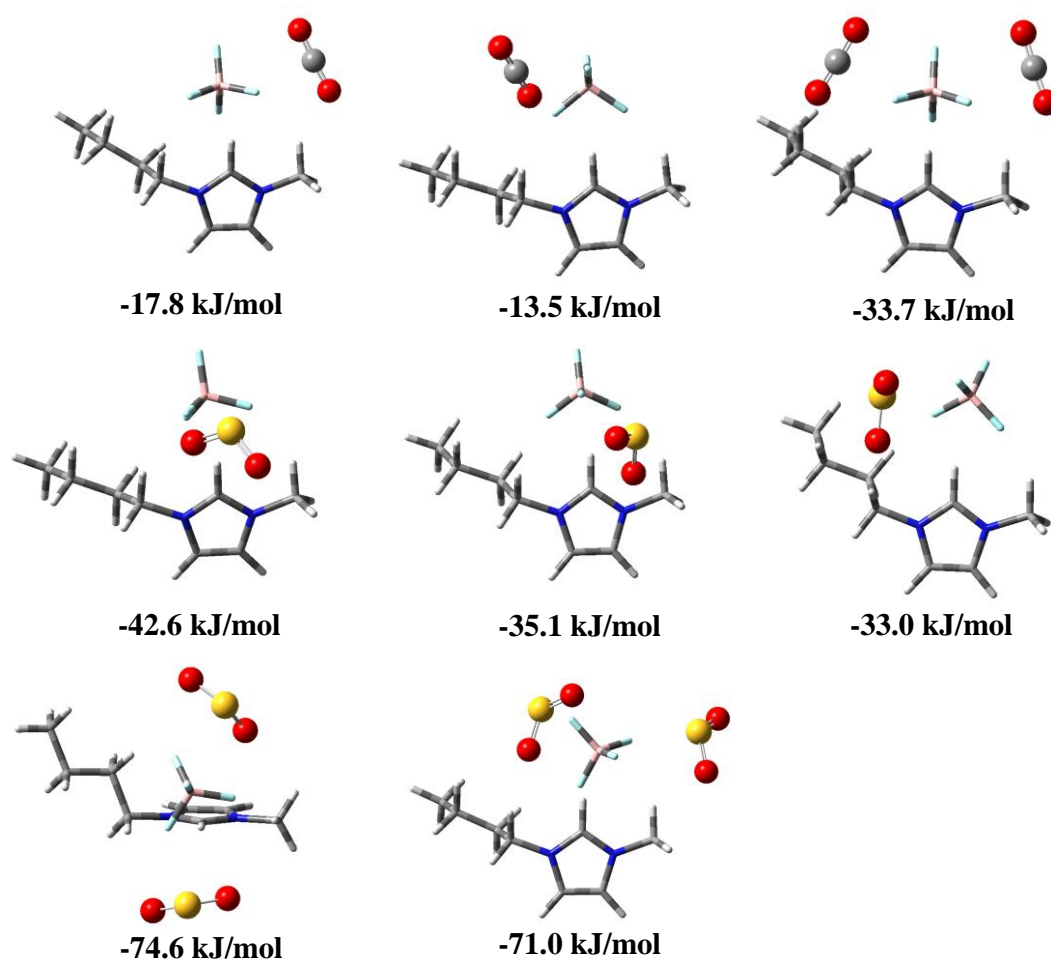


Figure S6. The optimized structures of [Bmim][BF₄]⁺CO₂ and [Bmim][BF₄]⁺SO₂. The shown values mean the binding energies between [Bmim][BF₄] and CO₂/SO₂.

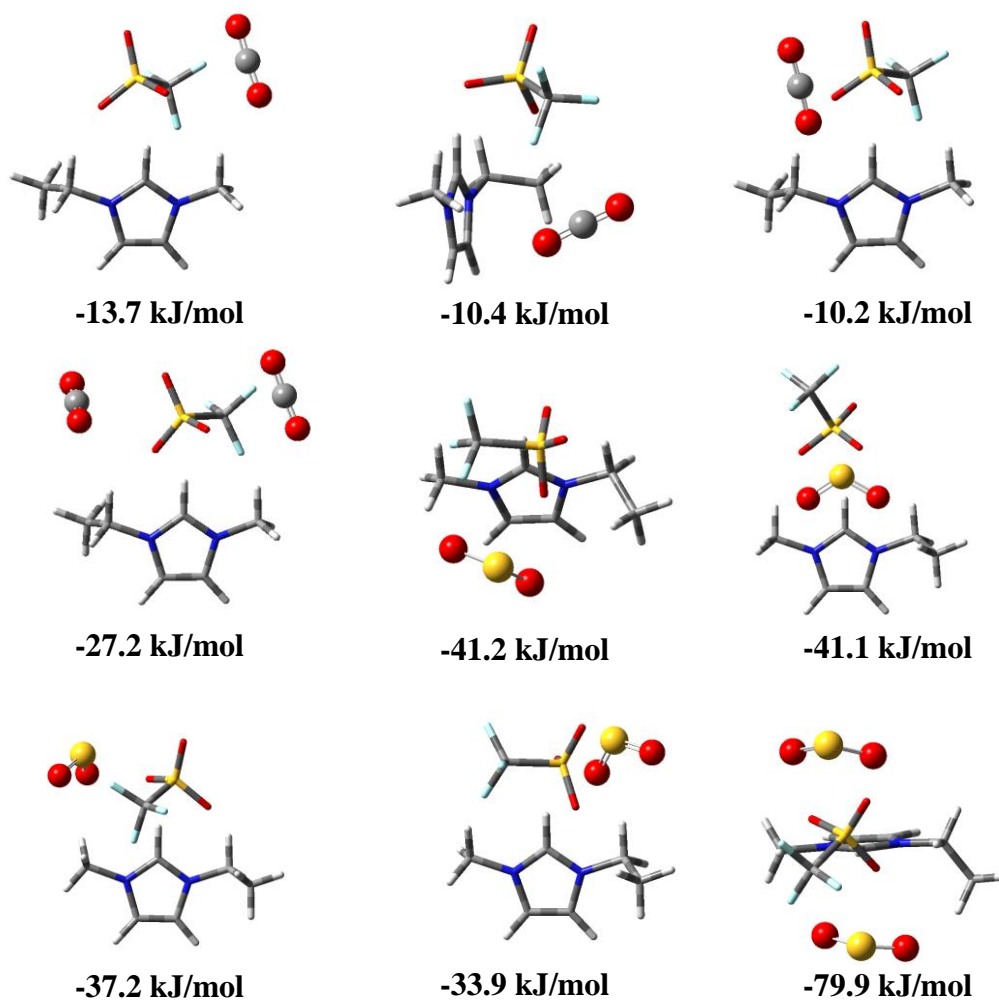


Figure S7. The optimized structures of [Emim][CF₃SO₃]⁺CO₂ and [Emim][CF₃SO₃]⁺SO₂. The shown values mean the binding energies between [Emim][CF₃SO₃] and CO₂/ SO₂.

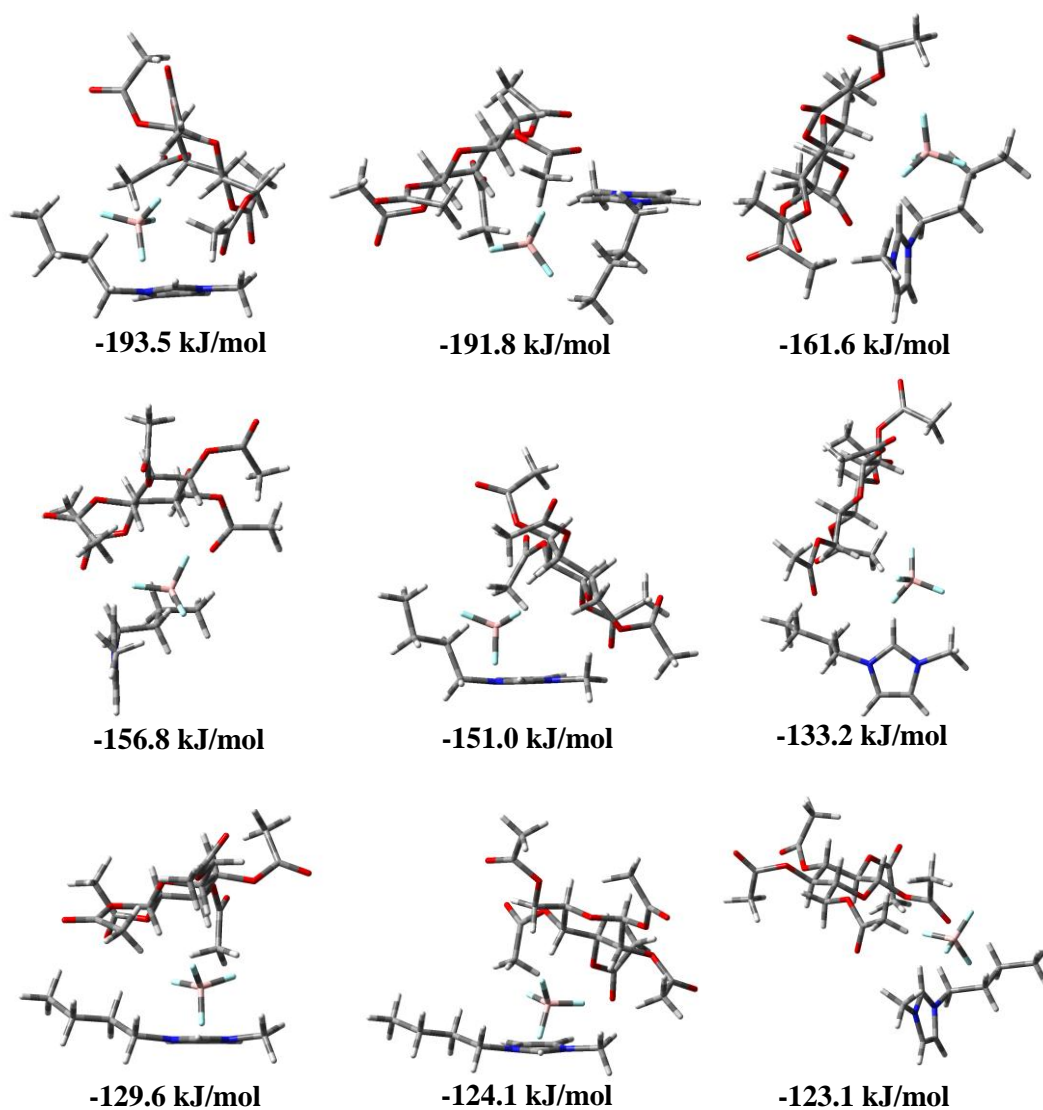


Figure S8. The optimized structures of [Bmim][BF₄]-GPA. The shown values mean the binding energies between [Bmim][BF₄] and GPA.

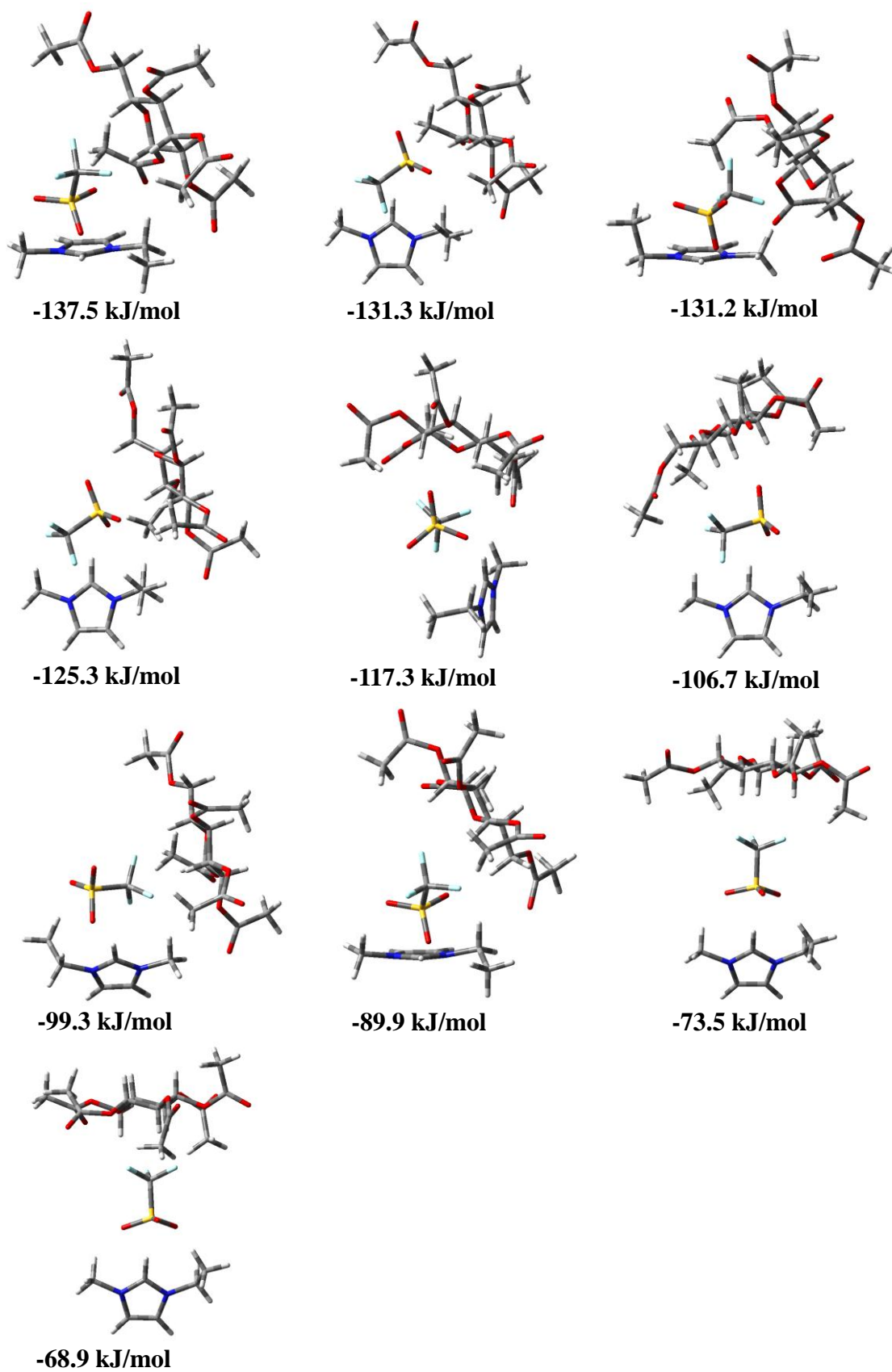


Figure S9. The optimized structures of [Emim][CF₃SO₃]-GPA. The shown values mean the binding energies between [Emim][CF₃SO₃] and GPA.

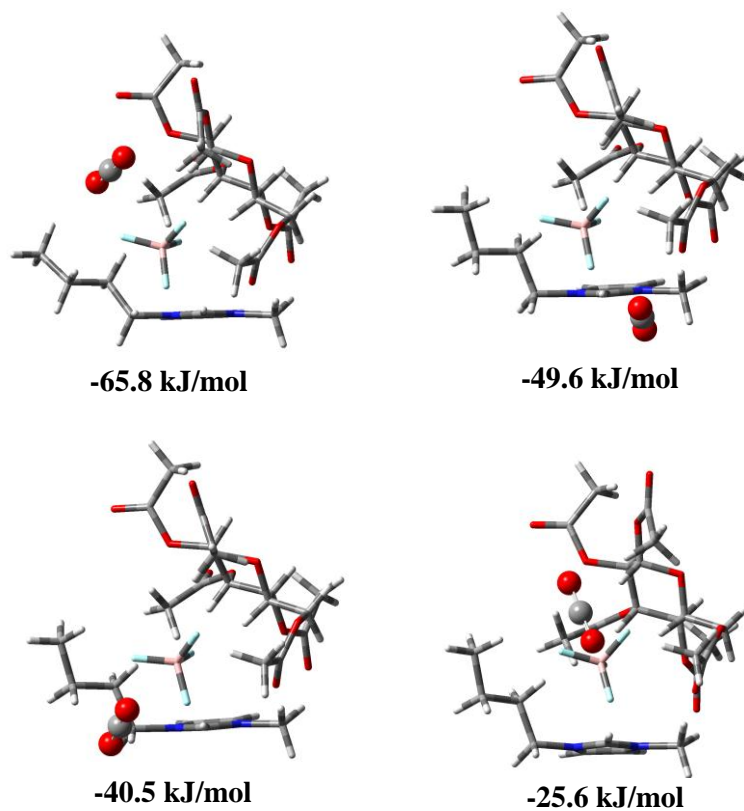


Figure S10. The optimized structures of [Bmim][BF₄]-GPA^{••}CO₂. The shown values mean the binding energies between CO₂ and the most stable [Bmim][BF₄]-GPA.

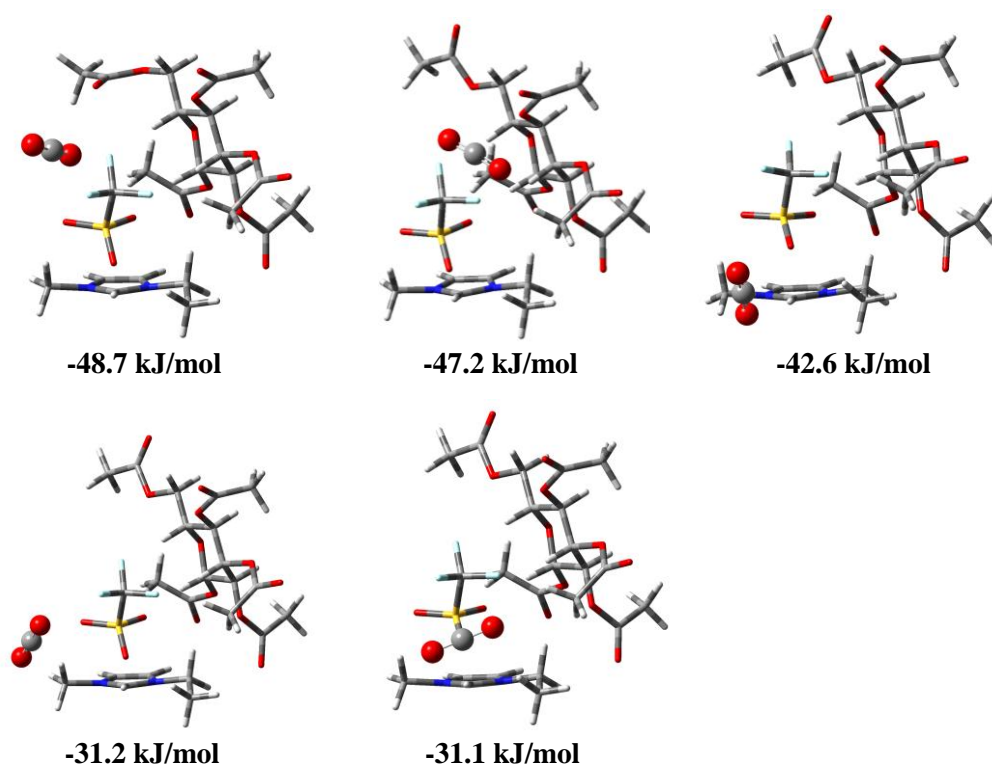


Figure S11. The optimized structures of [Emim][CF₃SO₃]-GPA⁺CO₂. The shown values mean the binding energies between CO₂ and the most stable [Emim][CF₃SO₃]-GPA.