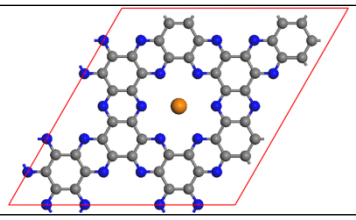
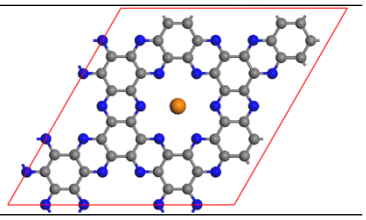
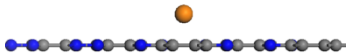
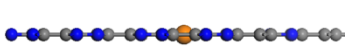
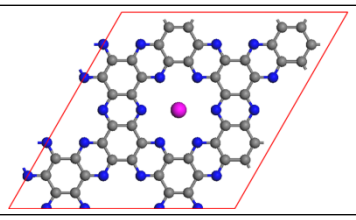
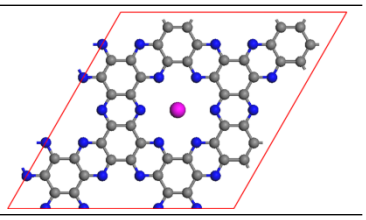
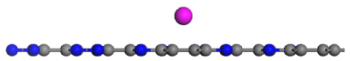
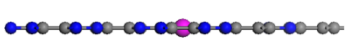
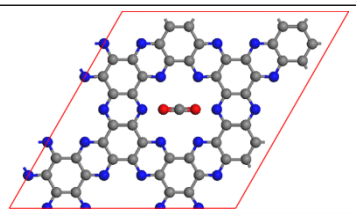
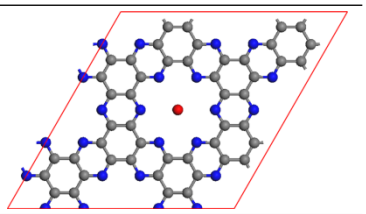
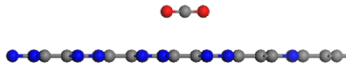
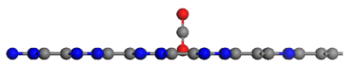
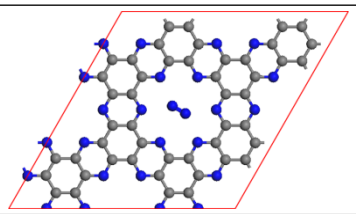
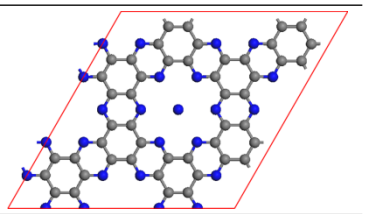
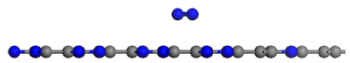
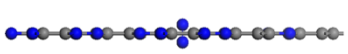
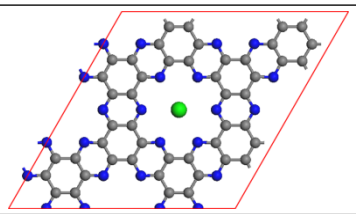
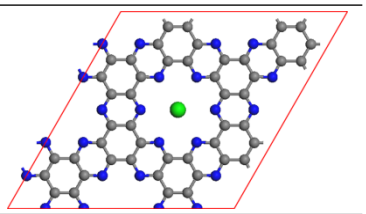
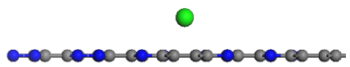
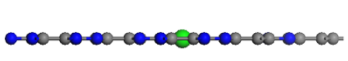
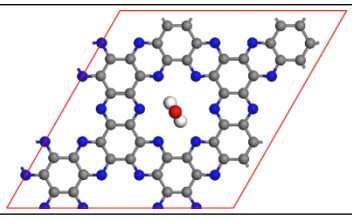
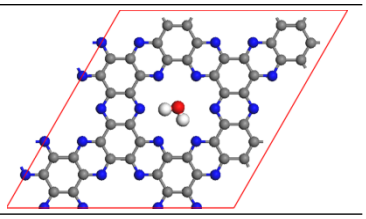
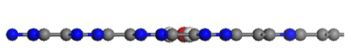
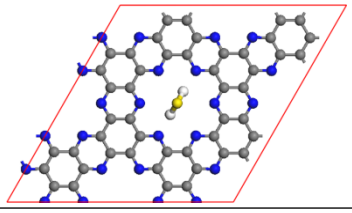
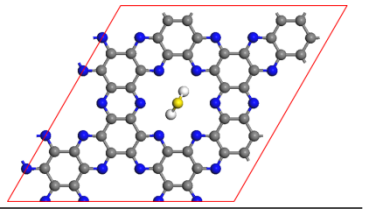
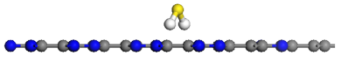
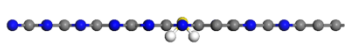
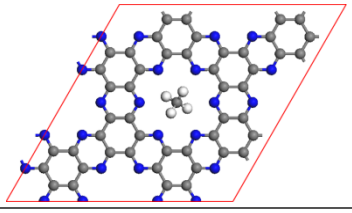
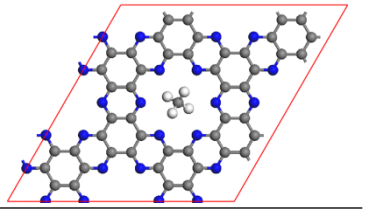
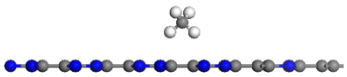
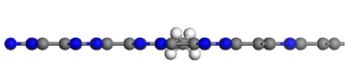
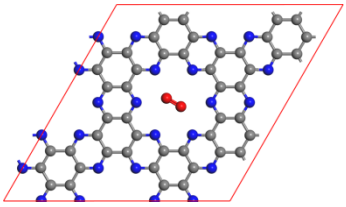
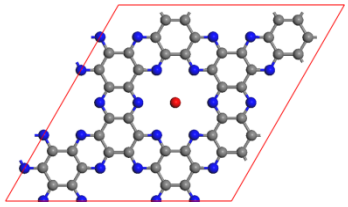
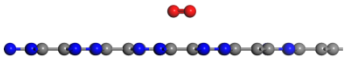
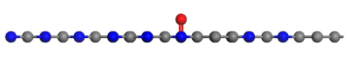
Table S1 The SS and TS for the studied gases passing through C_2N monolayer, and their interaction energies are in eV. Orange is He, magenta is Ne, green is Ar, gray is carbon, white is hydrogen and blue is nitrogen, red is oxygen, yellow is sulfur.

Gas	Property	Stable State	Transition State
He	Top View		
	Side View		
	Interaction Energy	-0.06 eV	0.07 eV
Ne	Top View		
	Side View		
	Interaction Energy	-0.08 eV	0.26 eV
CO_2	Top View		
	Side View		
	Interaction Energy	-0.19 eV	0.47 eV
N_2	Top View		
	Side View		
	Interaction Energy	-0.17 eV	0.70 eV
Ar	Top View		
	Side View		

	Interaction Energy	-0.09 eV	1.15 eV
H_2O	Top View		
	Side View		
	Interaction Energy	-0.59 eV	0.05 eV
H_2S	Top View		
	Side View		
	Interaction Energy	-1.20 eV	0.65 eV
CH_4	Top View		
	Side View		
	Interaction Energy	-0.07 eV	1.96 eV
O_2	Top View		
	Side View		
	Interaction Energy	-0.11 eV	0.68 eV

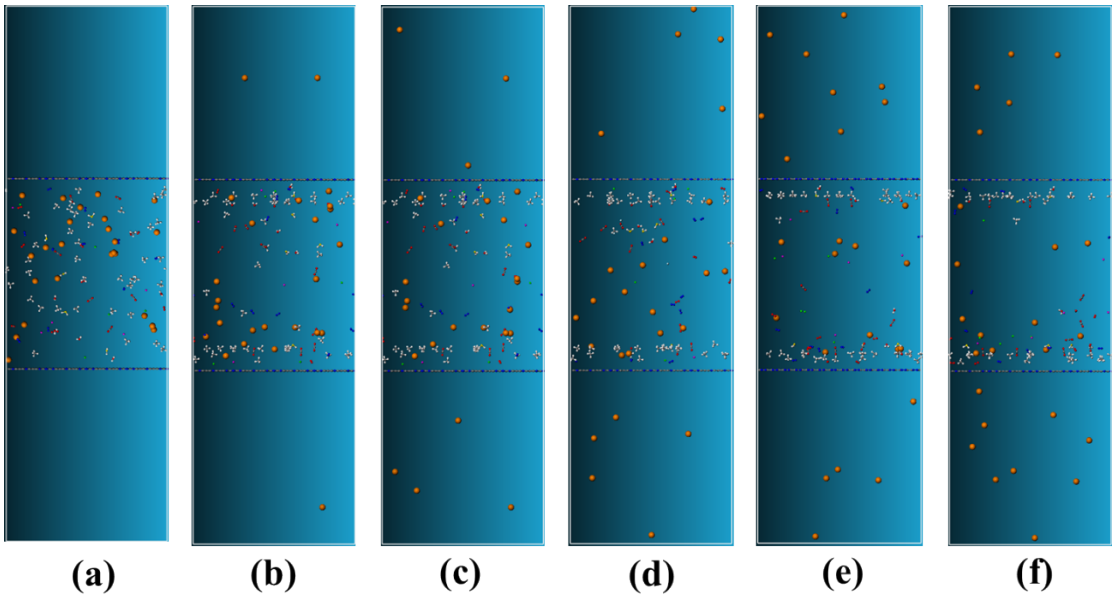


Fig. S1 Snapshots of configuration of the gas mixture permeating through C_2N monolayer at different temperatures. (a) the initial configuration, (b)-(f) the configuration after 1 ns simulation at different temperature. (b) 200 K, (c) 300 K, (d) 400 K, (e) 500 K and (f) 600 K. The C_2N monolayer was constructed with dimensions of 58.28 Å×57.67 Å.