

Supplementary Material

Table S1 The simulation models built in this work and their detailed information. Canonical ensemble runs at 350 K and 1 atm for all the models

System	Notation	Number of molecules			D_{GP} (Å)
		H ₂ O	SO ₂	O ₂	
A	A07	1924	40	20	7
	A10	1924	40	20	10
	A12	1924	40	20	12
	A15	1924	40	20	15
	B07	2101	---	---	7
B	B10	2101	---	---	10
	B12	2101	---	---	12
	B15	2101	---	---	15
	C	785	16	8	---

Table S2 The molar concentration of H₂O, SO₂ and O₂ molecules and the mass density within the double-layer graphene (DLG) for System A

Model	Molar concentration (%)			Mass density (g/cm ³)
	H ₂ O	SO ₂	O ₂	
A07	0.80	74.74	24.42	1.26
A10	3.11	66.05	30.83	0.98
A12	11.33	60.12	28.54	0.91
A15	45.23	36.58	18.19	0.80

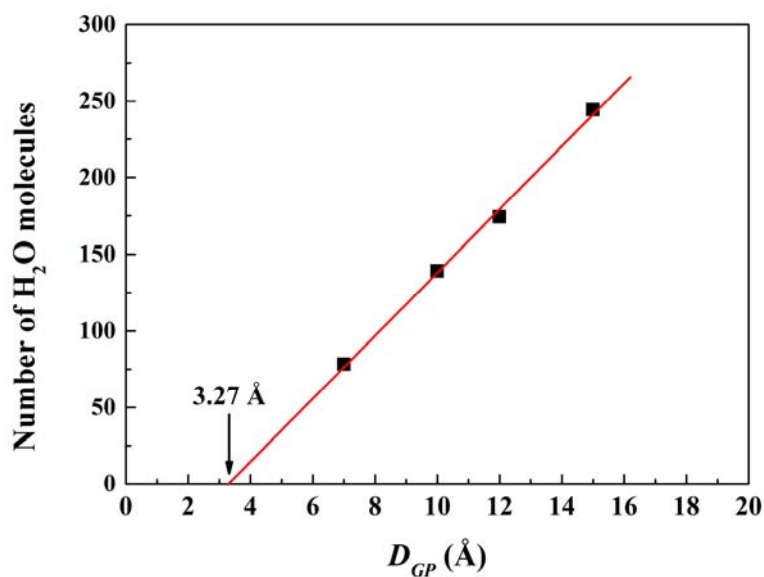


Fig. S1 The number of H₂O molecules inside the DLG in System B as the function of D_{GP} . The linear fit is represented as the red line, which has a threshold value of 3.27 Å

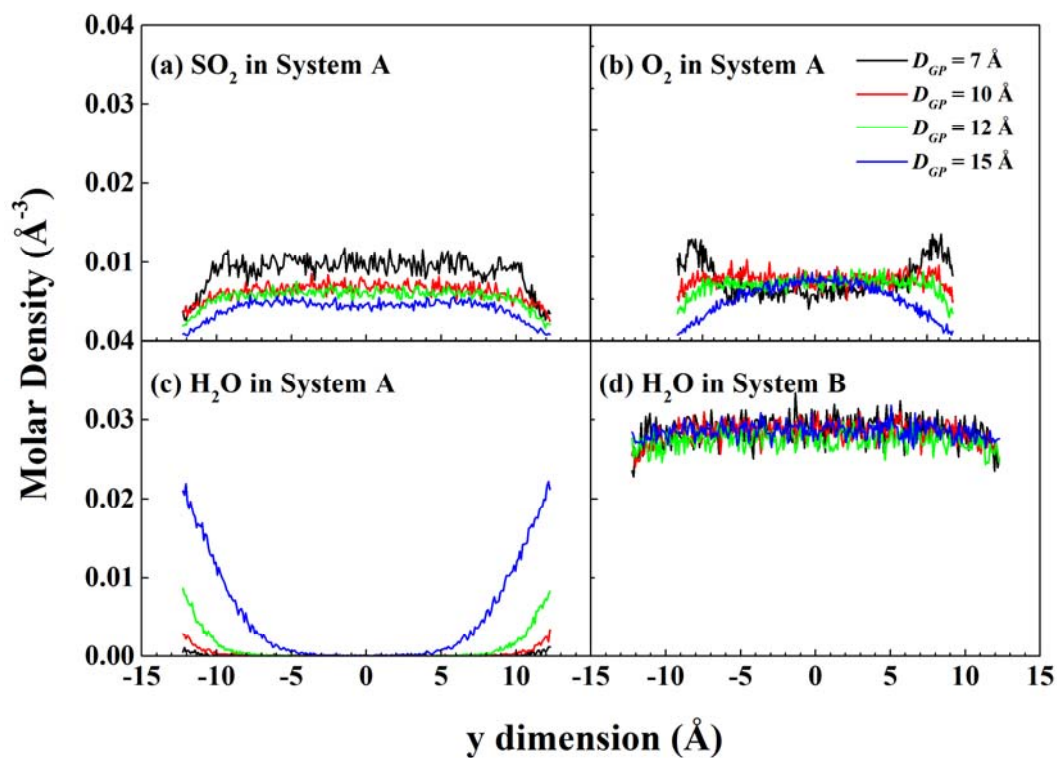


Fig. S2 The molar density along y axis for (a) H₂O, (b) O₂, (c) SO₂ within the DLG in System A and (d) H₂O in System B. The center of the DLG along y axis is aligned to zero

Table S3 The range of the nearest neighbor and the coordination number between H₂O, SO₂ and O₂

Central molecule	Coordinated molecule	Range of the nearest neighbor (Å)	Coordination number				
			A07	A10	A12	A15	C
H ₂ O	H ₂ O	3.48	4.70	4.79	4.84	4.88	4.91
	SO ₂	5.53	0.10	0.07	0.05	0.08	0.39
	O ₂	5.18	0.07	0.04	0.02	0.06	0.16
SO ₂	H ₂ O	5.53	4.61	3.32	2.44	3.84	19.13
	SO ₂	6.23	2.59	3.43	3.98	2.78	0.77
	O ₂	5.60	0.73	1.24	1.30	1.07	0.29
O ₂	H ₂ O	5.18	6.51	3.40	2.49	2.86	16.08
	SO ₂	5.60	1.46	2.48	2.60	2.14	0.58
	O ₂	5.58	1.24	1.19	1.29	1.18	0.24

* For System B, the coordination number of H₂O-H₂O pair is 4.74 for $D_{GP} = 7$ Å, 4.78 for $D_{GP} = 10$ Å, 4.79 for $D_{GP} = 12$ Å and 4.78 for $D_{GP} = 15$ Å

Table S4 The retention time of the coordinated molecular pairs between H₂O, SO₂ and O₂

Pair of coordinated molecules	Retention time (ps)				
	A07	A10	A12	A15	C
H ₂ O – H ₂ O	4.22	4.21	4.23	4.43	4.47
H ₂ O – SO ₂	5.88	6.00	6.08	5.52	6.68
H ₂ O – O ₂	4.78	5.14	5.61	5.12	6.26
SO ₂ – SO ₂	12.27	9.34	7.57	6.31	13.94
SO ₂ – O ₂	9.63	6.58	5.25	4.95	10.52
O ₂ – O ₂	8.35	6.66	5.54	4.15	8.76

* For System B, the lifetime of H₂O-H₂O pair is 4.44 ps for $D_{GP} = 7 \text{ \AA}$, 4.34 ps for $D_{GP} = 10 \text{ \AA}$, 4.23 ps for $D_{GP} = 12 \text{ \AA}$ and 4.31 ps for $D_{GP} = 15 \text{ \AA}$

Table S5 The average number of hydrogen bonds in System A and C

	Average number of hydrogen bond				
	System A07	System A10	System A12	System A15	System C
O _w -H _w ...O _w	3.26	3.28	3.28	3.29	3.32
O _w -H _w ...O _s	0.18	0.14	0.10	0.16	0.56
O _w -H _w ...O	0.11	0.05	0.05	0.05	0.19

Table S6 The diffusion coefficient and their components for System A, B and C

Molecule	Component	Diffusion coefficient ($10^{-5} \text{ cm}^2/\text{s}$)				
		A07	A10	A12	A15	C*
H ₂ O	<i>D</i>	5.94	5.65	5.58	5.44	5.86
	<i>D_x</i>	2.41	2.29	2.21	2.37	1.95
	<i>D_y</i>	2.00	1.88	1.86	1.73	1.95
	<i>D_z</i>	1.54	1.48	1.51	1.34	1.95
SO ₂	<i>D</i>	3.82	6.21	7.13	5.37	2.55
	<i>D_x</i>	3.16	5.74	6.9	5.25	0.85
	<i>D_y</i>	0.42	0.89	0.17	0.06	0.85
	<i>D_z</i>	0.24	0.18	0.06	0.06	0.85
O ₂	<i>D</i>	6.74	7.37	6.01	9.12	4.62
	<i>D_x</i>	4.60	6.30	5.61	8.52	1.54
	<i>D_y</i>	2.39	0.32	0.32	0.42	1.54
	<i>D_z</i>	0.47	0.15	0.12	0.18	1.54
		B07	B10	B12	B15	
H ₂ O	<i>D</i>	5.82	5.70	5.58	5.84	
	<i>D_x</i>	2.33	2.35	2.14	2.34	
	<i>D_y</i>	2.12	2.08	2.13	2.18	
	<i>D_z</i>	1.37	1.27	1.31	1.33	

* For System C, the *x*, *y* and *z* components of the diffusion coefficient are equal