Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information

Mechanistic Insights into CO_2 Activation on Pristine, Defected and Doped Goldene: A Single-Atom Layer of Gold

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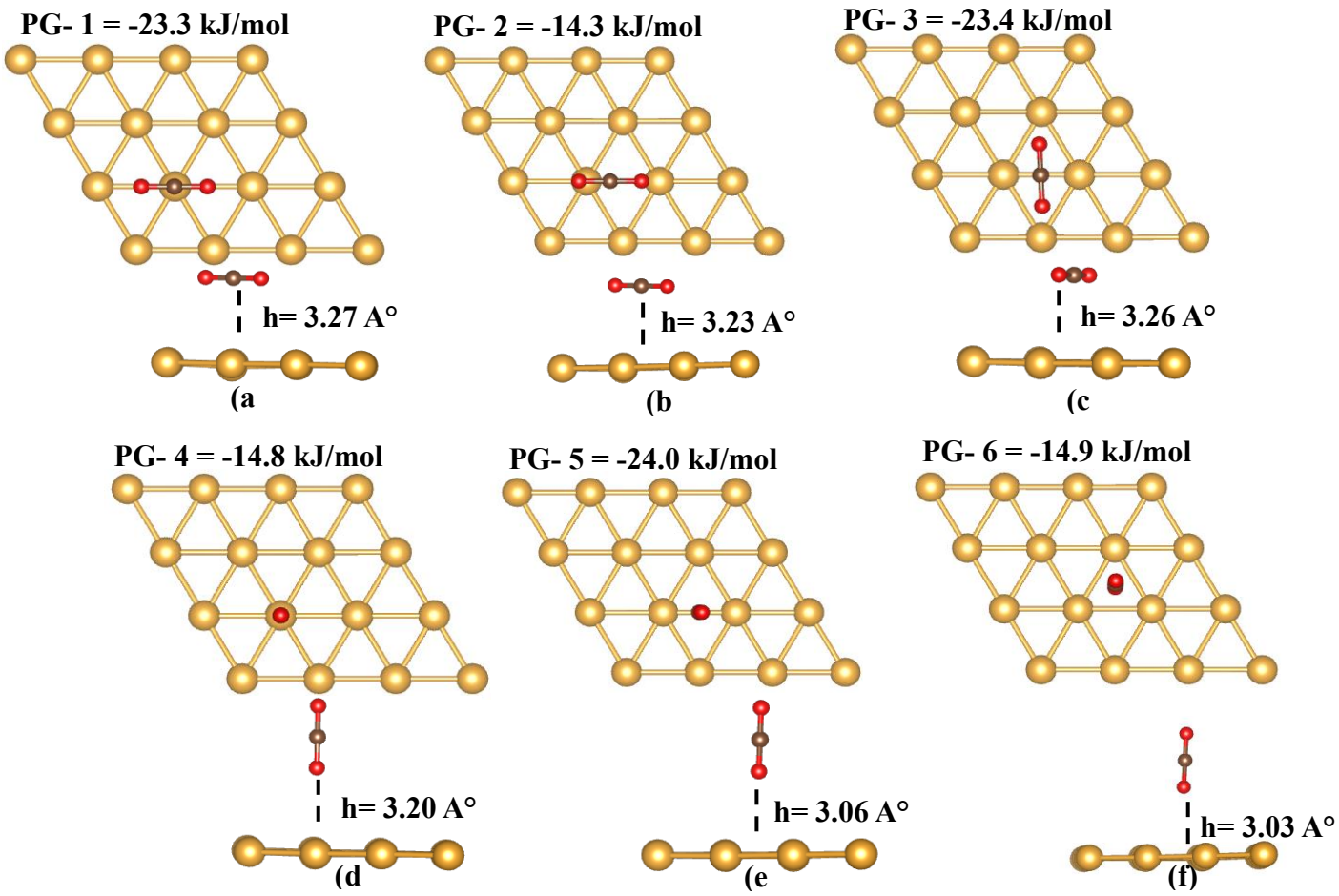

Figure S1. Top and side view of optimized geometries of CO_2 at 4×4×1 supercell

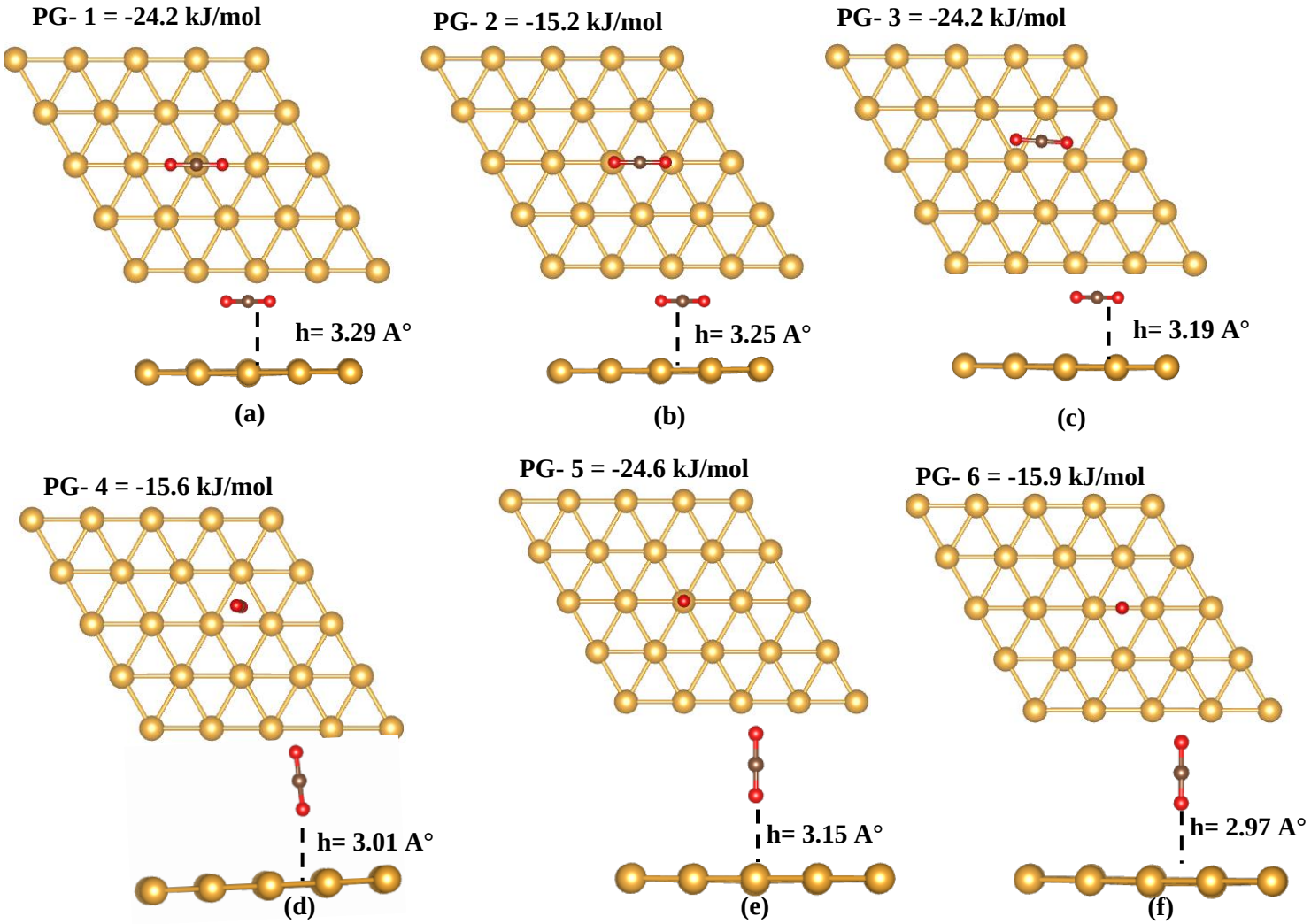

Figure S2. Top and side view of optimized geometries of CO_2 at 5×5×1 supercell

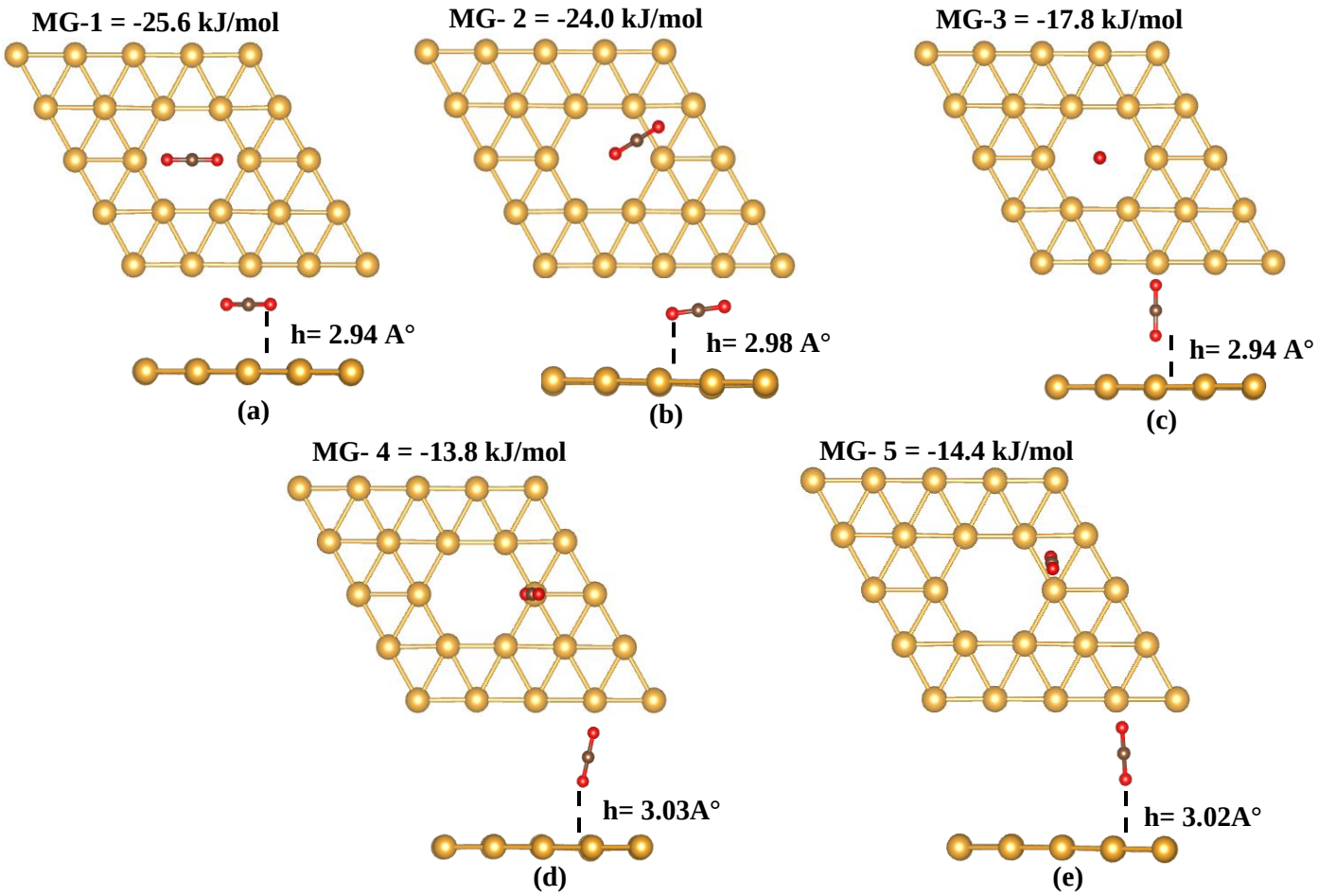

Figure S3. Top and side view of optimized geometries of CO_2 at MG supercell

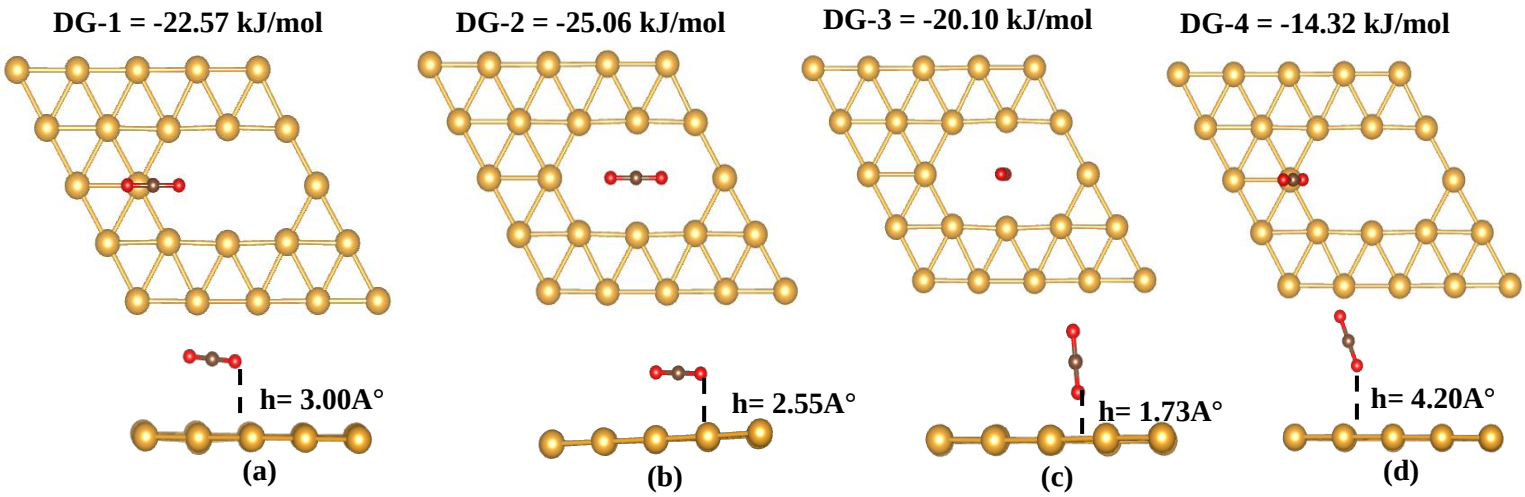

Figure S4. Top and side view of optimized geometries of CO_2 at DG supercell

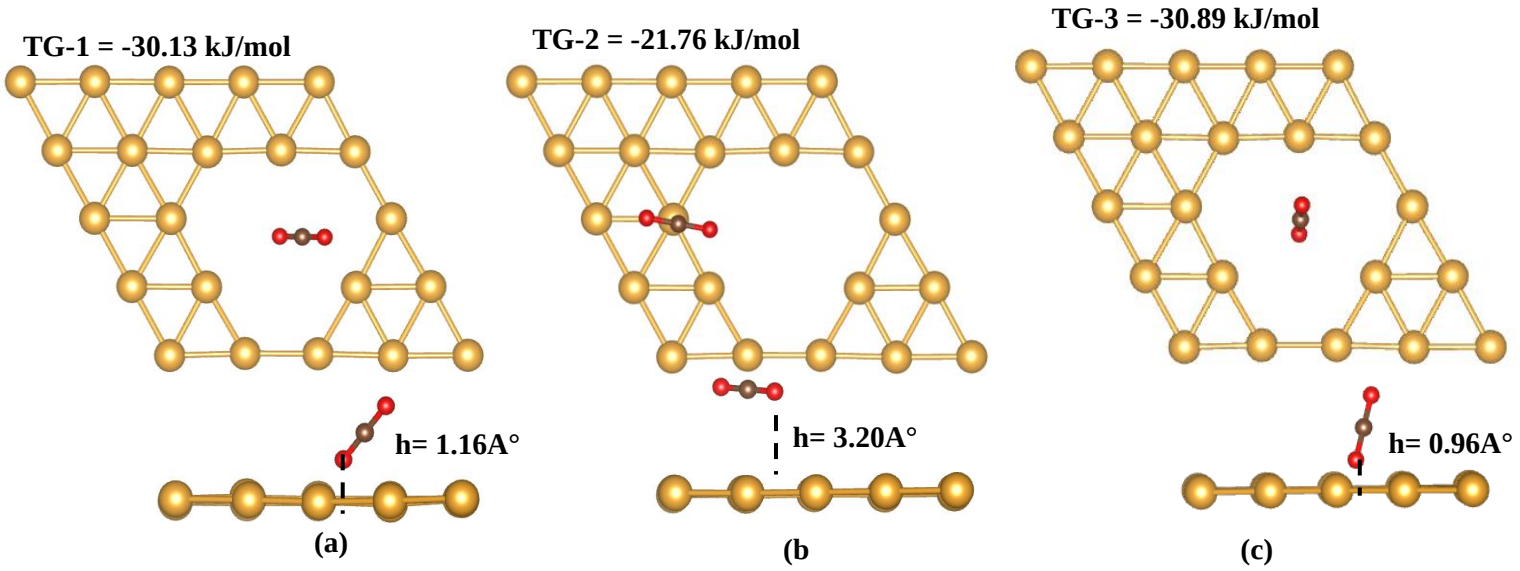

Figure S5. Top and side view of optimized geometries of CO_2 at TG supercell

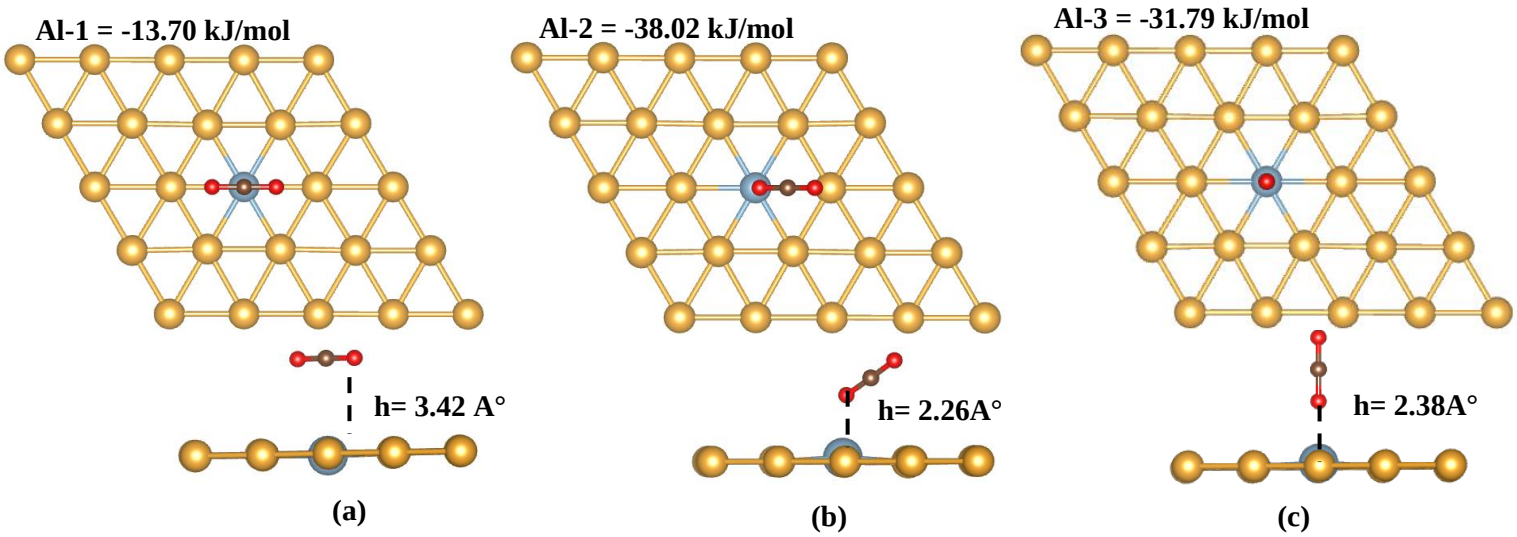

Figure S6. Top and side view of optimized geometries of CO_2 at Al@PG supercell

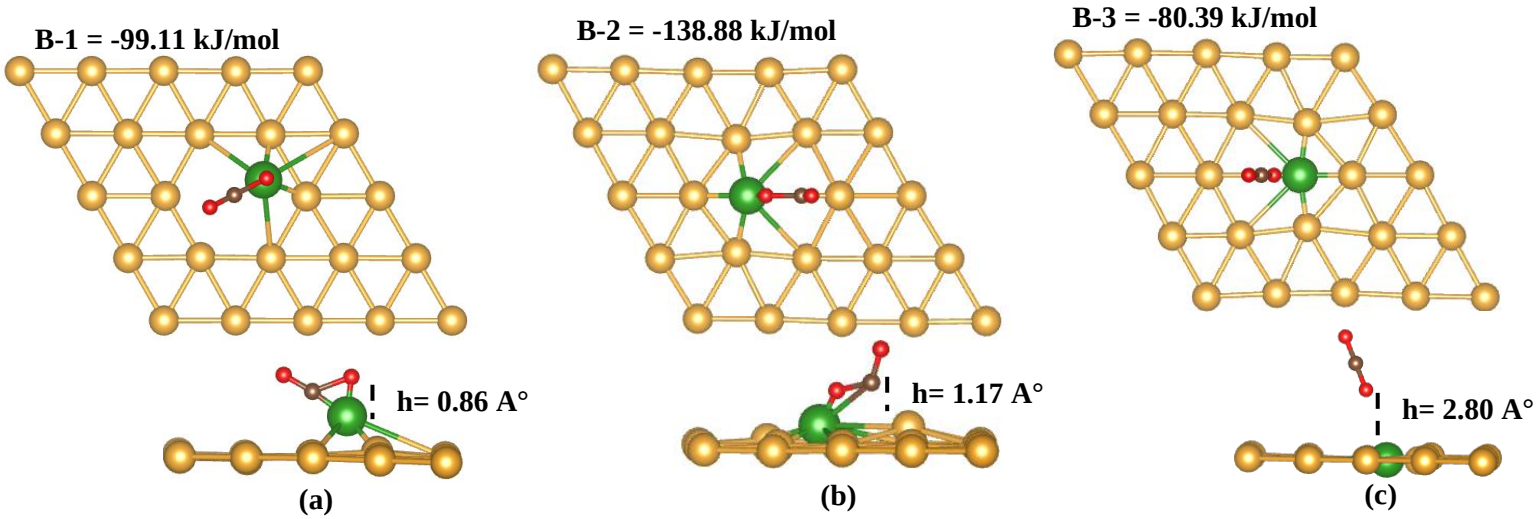

Figure S7. Top and side view of optimized geometries of CO_2 at B@PG supercell

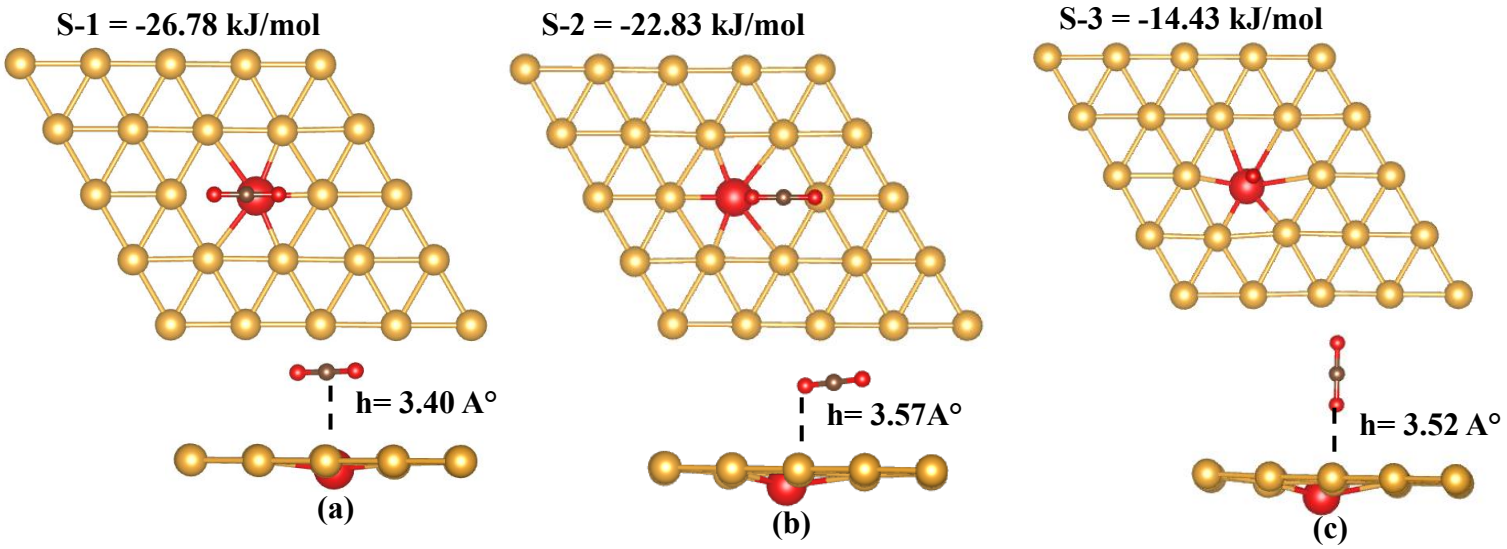

Figure S8. Top and side view of optimized geometries of CO_2 at S@PG supercell

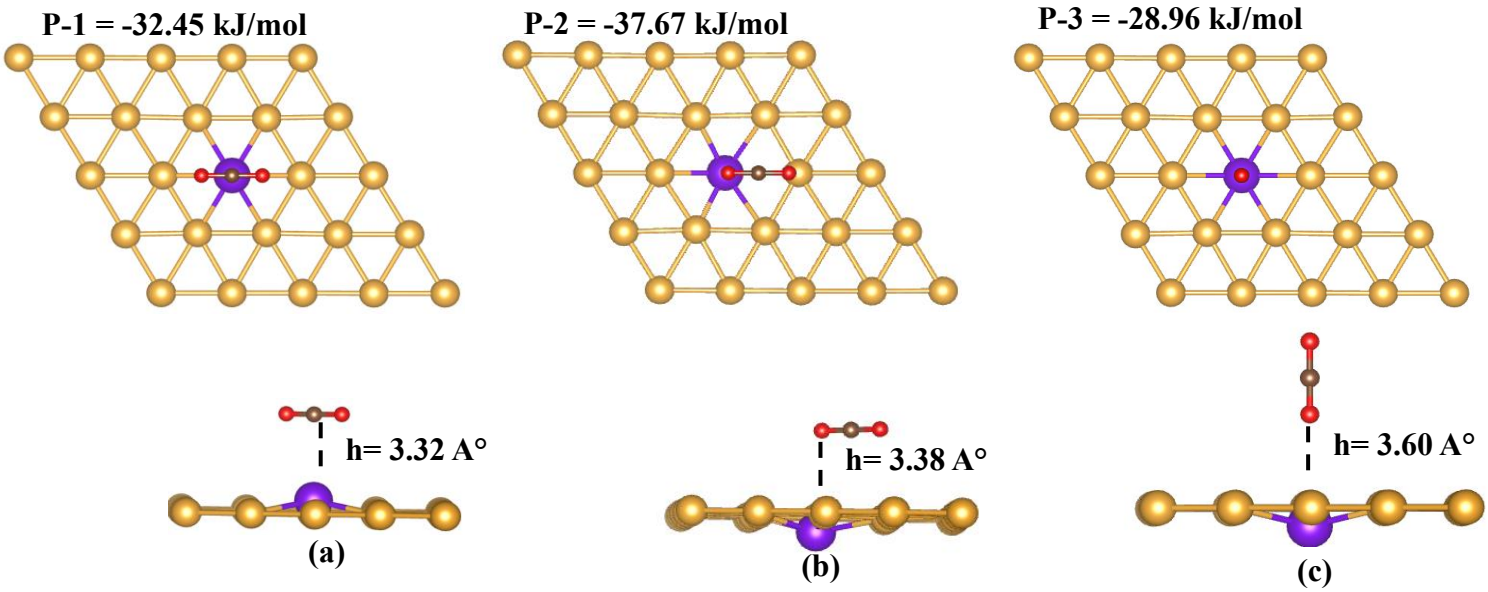

Figure S9. Top and side view of optimized geometries of CO_2 at P@PG supercell

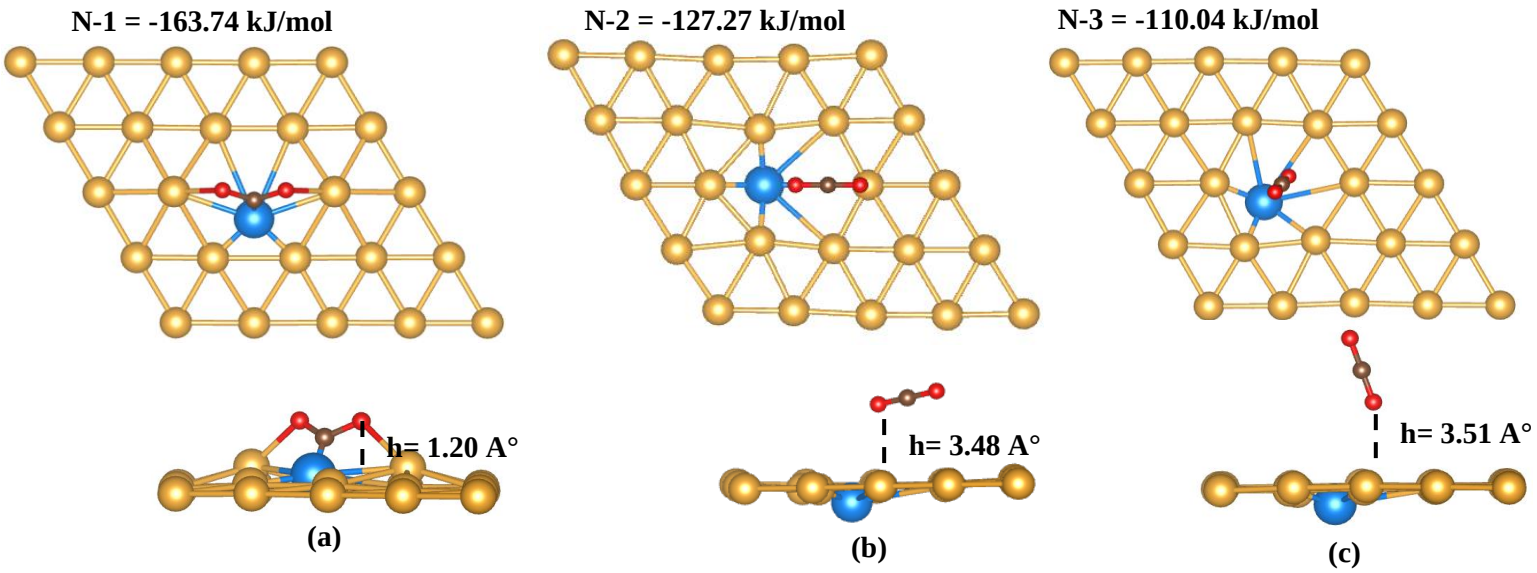

Figure S10. Top and side view of optimized geometries of CO_2 at N@PG supercell

Table S1 Adsorption energy E_{ad_PG} (kJ/mol), adsorption height h (Å), bond length l (Å) and bond angle of CO_2 molecule θ() for CO_2@PG system

Conf.		4×4×1					5×5×1				
		E_{ad_PG}	h	l		θ	E_{ad_PG}	h	l		θ
				Au-Au	C-O				Au-Au	C-O	
A	∥(PG-1)	-23.3	3.27	2.74	1.17	179.6°	-24.2	3.29	2.75	1.17	179.9°
	⊥(PG-2)	-14.3	3.23	2.74	1.17	179.8°	-15.2	3.25	2.74	1.17	179.8°
B	∥(PG-3)	-23.4	3.26	2.74	1.17	179.8°	-24.2	3.19	2.74	1.17	179.9°
	⊥(PG-4)	-14.8	3.20	2.74	1.18	179.9°	-15.6	3.01	2.74	1.17	179.9°
C	∥(PG-5)	**-24.0**	**3.06**	**2.74**	**1.18**	**179.9°**	**-24.6**	**3.15**	**2.74**	1.18	179.9°
	⊥(PG-6)	-14.9	3.03	2.74	1.18	179.8°	-15.9	2.97	2.75	1.18	179.9°

Table S2 Calculated adsorption energy E_{ad_def} (kJ/mol), adsorption height h (Å), bond length l (Å), bond angle θ, of defected goldene after CO_2 adsorption.

		E_{ad_def}	h	L		θ
				Au-Au	C-O	
MG	**MG-1**	**-25.6**	**2.94**	**2.68-2.76**	**1.17**	**179.8°**
	MG-2	-24.0	2.98	2.69-2.75	1.17	179.5°
	MG-3	-17.8	2.94	2.69-2.75	1.18	179.9°
	MG-4	-13.8	3.03	2.68-2.76	1.18	179.8°
	MG-5	-14.4	3.02	2.69-2.73	1.17	179.9°
DG	**DG-1**	-22.57	3.00	2.69-2.77	1.18	179.5°
	DG-2	**-25.06**	**2.55**	**2.69-2.77**	**1.18**	**179.8°**
	DG-3	-20.10	1.73	2.69-2.80	1.18	179.9°
	DG-4	-14.32	4.20	2.70-2.77	1.17	179.7°
TG	**TG-1**	-30.13	1.16	2.68-2.81	1.18	179.7°
	TG-2	-21.76	3.20	2.68-2.78	1.17	179.8°
	TG-3	**-30.89**	**0.96**	**2.68-2.76**	**1.18**	**179.7°**

Table S3 Optimized parameters of CO_2 adsorbed X@PG systems along with adsorption energies E_{aX} (kJ/mol), adsorption height h(Å), bond lengths l(Å) and bond angle θ

X	Conf.	E_{aX}	H	l			θ
				Au-Au	C-O	Au-X	
Al	Al-1	-13.70	3.42	2.76	1.17	2.68	178.9°
	Al-2	**-38.02**	**2.66**	**2.76**	**1.19**	**2.69**	178.6°
	Al-3	-31.79	2.38	2.74	1.18	2.69	178.9°
B	B-1	-99.11	0.86	2.79	1.48	2.16	129.6°
	B-2	**-138.88**	**1.17**	**2.92**	**1.39**	**3.35**	**119.9°**
	B-3	-80.39	2.80	2.98	1.18	3.58	179.7°
S	**S-1**	**-26.78**	**3.40**	**2.75**	**1.17**	**2.99**	**179.0°**
	S-2	-22.83	3.57	2.76	1.17	3.22	179.7°
	S-3	-14.43	3.52	2.78	1.18	3.40	179.9°
P	P-1	-32.45	3.32	2.77	1.18	2.72	178.9°
	P-2	**-37.67**	3.38	2.75	1.17	2.90	179.9°
	P-3	-28.96	3.60	2.80	1.17	2.74	179.9°

N	**N-1**	**-163.74**	**1.20**	**2.90**	**1.28**	**3.59**	**120.9°**
	N-2	-117.27	3.48	2.99	1.17	3.48	179.7°
	N-3	-110.04	3.51	2.78	1.17	3.70	179.9°

Table S4 Bader charge analysis of amount of charge transfer on dopants (X= Al, B, S, P, N) and CO_2 molecule during the process of doping and adsorption

System	**X**	**C**	**O**	**CO_2**
Al@PG	2.93	---	---	---
B@PG	0.18	---	---	---
S@PG	-0.38	---	---	---
P@PG	-0.04	---	---	---
N@PG	-0.52	---	---	---
CO_2+PG (PG-5)	---	3.99	-2.01, -2.00	-0.02
CO_2+MG (MG-1)	---	3.99	-1.98, -2.05	-0.04
CO_2+DG (DG-2)	---	3.99	-2.01, -2.03	-0.05
CO_2+TG (TG-3)	---	3.99	-2.03, -2.01	-0.05
CO_2+ Al@PG (Al-2)	2.93	3.99	-1.98, -2.10	-0.09
CO_2+ B@PG (B-2)	1.37	2.54	-1.86, -1.90	-1.22
CO_2+ S@PG (S-1)	-0.35	3.99	-2.01, -2.01	-0.03
CO_2+ P@PG (P-2)	0.07	3.99	-2.01, -2.00	-0.02
CO_2+ N@PG (N-1)	-1.76	3.99	-1.65, -1.68	0.66