Supporting information for

Nitrogen and Boron coordinated single-atom catalysts for Low-temperature CO/NO oxidations

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Table S1. The adsorption heights (d_1, Å), bond distance (d_2, Å), amount of transfer charge between metal Co atoms and reactive gas species ($\Delta q_1/\Delta q_2$, e).

Substrates	Gas reactants					
	CO	NO	O_2	O	CO_2	NO_2
	d_1, d_2	d_1, d_2	d_1, d_2	d_1	d_1, d_2	d_1, d_2
	Δq_1, Δq_2	Δq_1, Δq_2	Δq_1, Δq_2	Δq_1, Δq_2	Δq_1, Δq_2	Δq_1, Δq_2
B_1-gra-Co	1.87, 1.15	1.71, 1.18	1.88, 1.37	1.63	2.01, 1.18	1.81, 1.40
	0.57, 0.19	0.68, 0.36	0.78, 0.66	0.82, 0.71	0.56, 0.03	0.70, 0.65
B_2-gra-Co	1.82, 1.15	1.67, 1.18	1.88, 1.36	1.63	2.00, 1.18	1.78, 1.37
	0.34, 0.21	0.46, 0.31	0.58, 0.62	0.60, 0.70	0.27, 0.02	0.51, 0.64
B_3-gra-Co	1.82, 1.15	1.67, 1.17	1.85, 1.37	1.64	1.97, 1.18	1.83, 1.37
	0.17, 0.19	0.28, 0.27	0.48, 0.63	0.47, 0.65	0.14, 0.02	0.29, 0.61
N_1-gra-Co	1.87, 1.16	1.72, 1.20	1.80, 1.37	1.60	2.27, 1.18	1.79, 1.39
	0.89, 0.24	0.97, 0.46	1.12, 0.75	1.12, 0.73	0.92, 0.03	1.08, 0.60
N_2-gra-Co	1.82, 1.17	1.65, 1.20	1.80, 1.39	1.61	2.22, 1.18	1.80, 1.39
	0.99, 0.31	1.03, 0.45	1.19, 0.77	1.19, 0.72	0.97, 0.05	1.14, 0.63
N_3-gra-Co	1.77, 1.17	1.64, 1.20	1.82, 1.38	1.62	2.04, 1.19	1.84, 1.38
	1.01, 0.38	1.09, 0.48	1.25, 0.71	1.25, 0.72	1.04, 0.07	1.23, 0.70
B_1N_1-gra-Co	1.82, 1.16	1.65, 1.19	1.80, 1.37	1.62	2.16, 1.18	1.77, 1.39
	0.63, 0.28	0.74, 0.41	0.82, 0.67	0.86, 0.71	0.61, 0.03	0.77, 0.61
B_1N_2-gra-Co	1.71, 1.17	1.64, 1.19	1.82, 1.38	1.61	2.12, 1.18	1.77, 1.41
	0.64, 0.37	0.77, 0.42	0.83, 0.71	0.93, 0.74	0.70, 0.04	0.84, 0.61
B_2N_1-gra-Co	1.73, 1.16	1.66, 1.19	1.78, 1.37	1.62	2.01, 1.18	1.95, 1.31
	0.32, 0.24	0.56, 0.40	0.66, 0.67	0.61, 0.70	0.35, 0.02	0.56, 0.62
SV-gra-Co	1.88, 1.16	1.74, 1.20	1.90, 1.37	1.61	2.19, 1.18	1.78, 1.40
	0.83, 0.21	0.93, 0.45	1.04, 0.68	1.06, 0.74	0.86, 0.03	1.01, 0.63

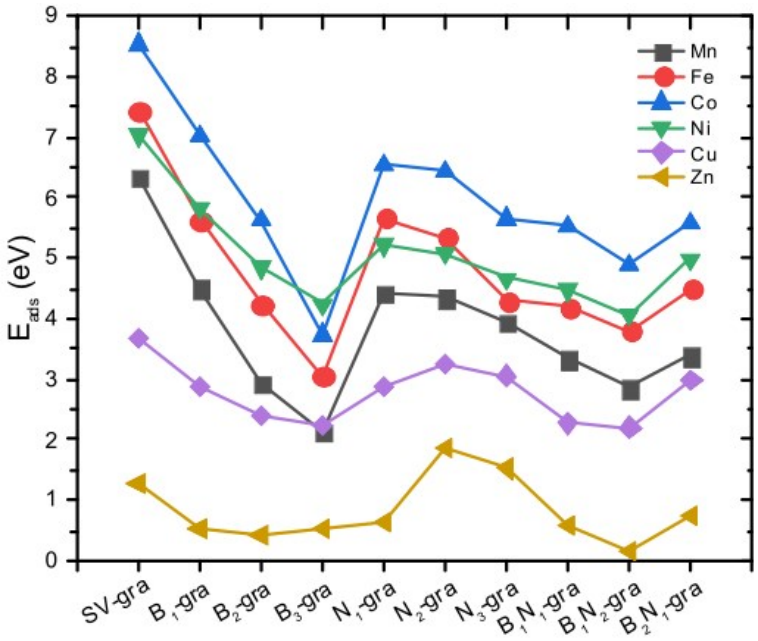

Fig.S1. The adsorption stability for transition metal atoms (M=Mn, Fe, Co, Ni, Cu and Zn) anchored B_xN_y-graphene sheets.

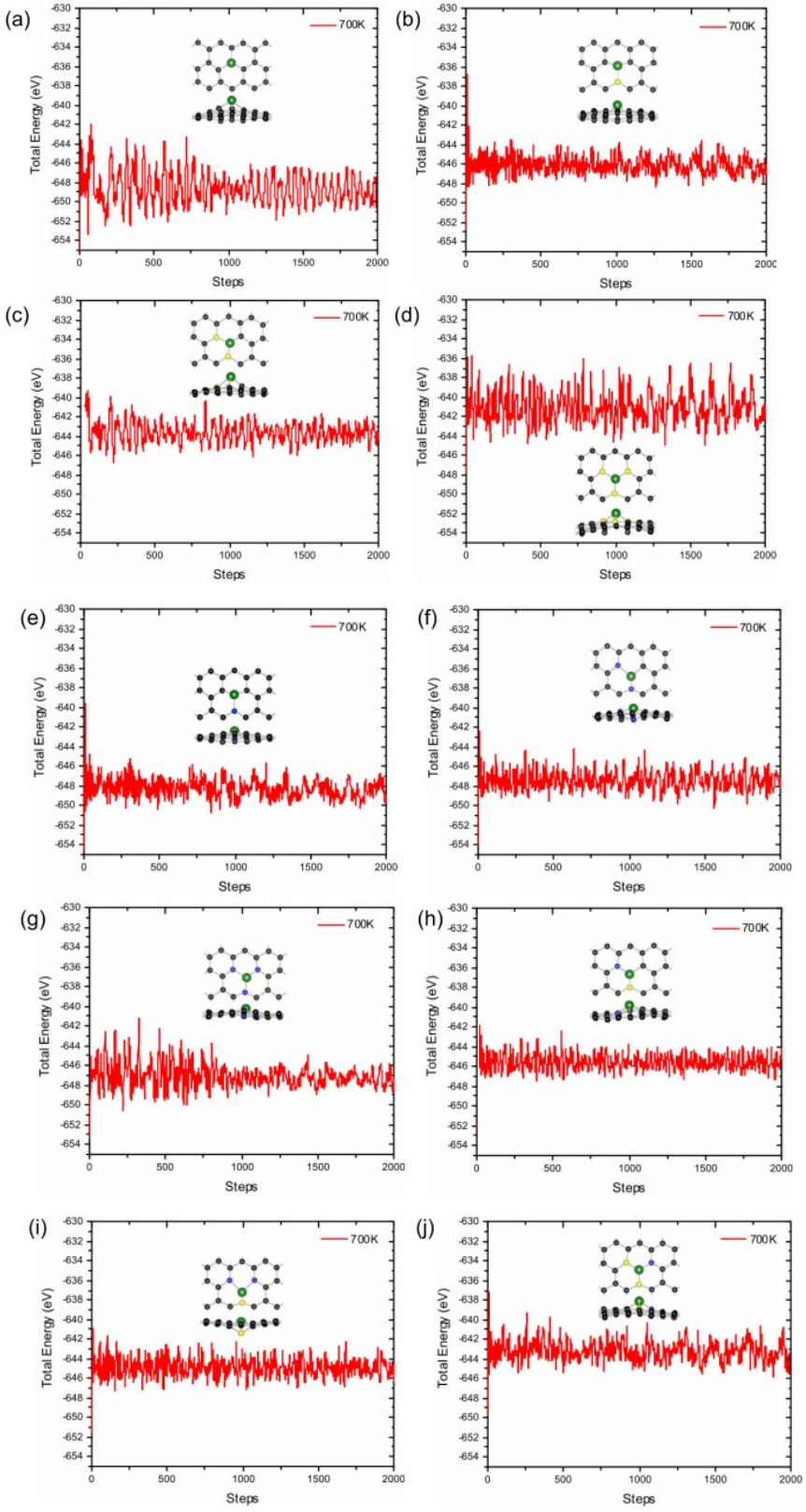

Fig.S2. The formation of (a) SV-graphene-Co and (b)-(j) B_xN_y-graphene-Co configurations from the molecular dynamics simulation at 700 K.

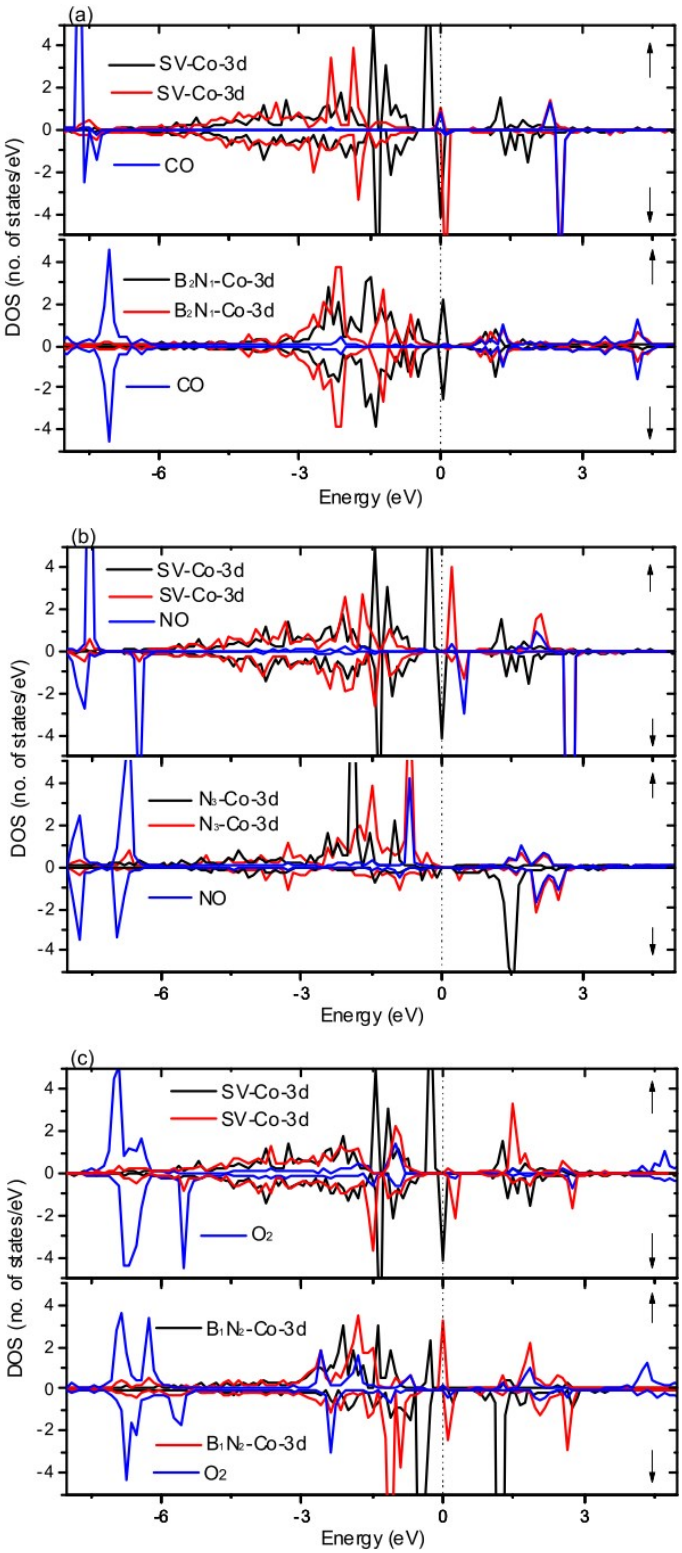

Fig.S3. The DOS plots for (a) CO, (b) NO and (c) O_2 adsorbed SV-graphene-Co and B_xN_y-graphene-Co sheets, the black, red and blue curves represent the PDOS of Co-*3d* orbitals without (or with) gas adsorption and the LDOS of adsorbed gases.

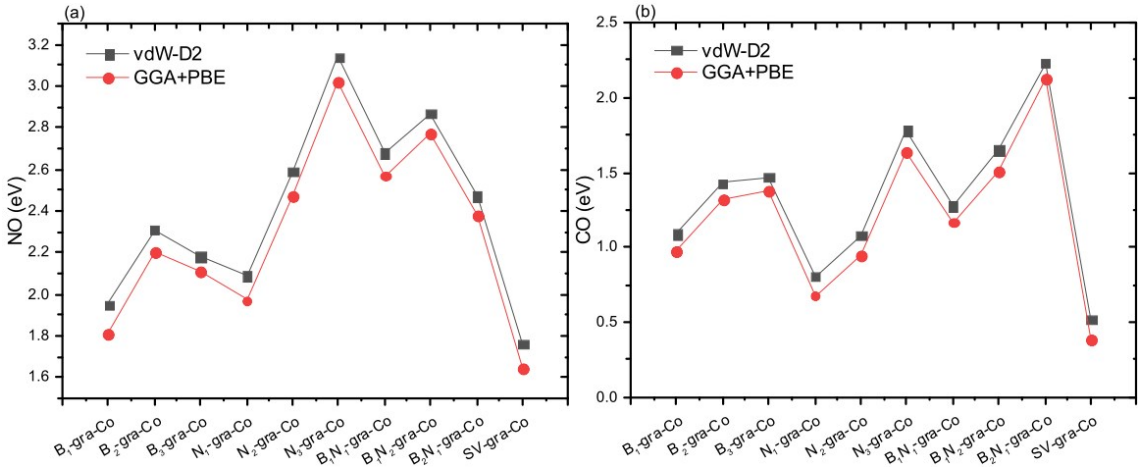

Fig.S4. The trend of adsorption stability for (a) NO and (b) CO on different graphene substrates by the GGA + PBE and vdW-D2 calculations.

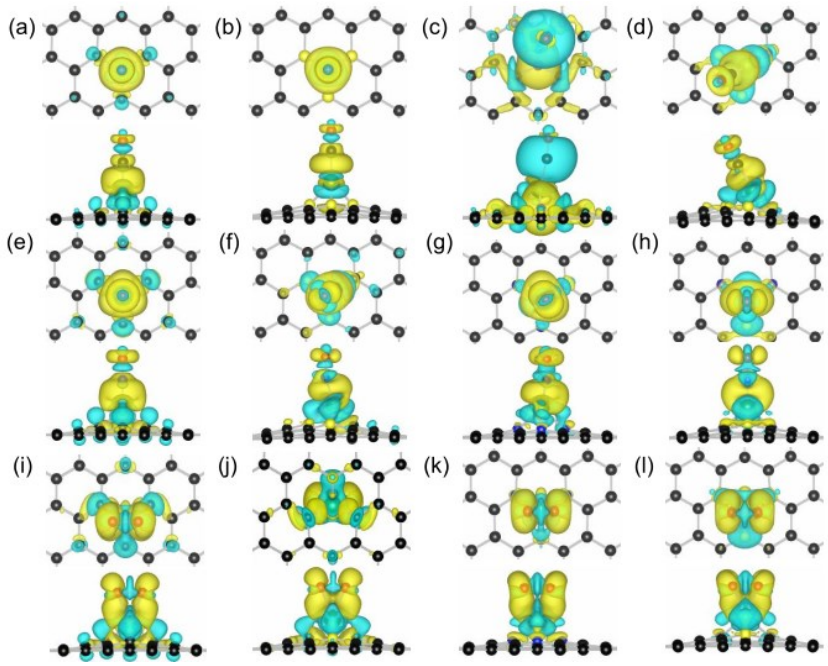

Fig.S5. Charge density difference plots for (a)-(d) CO, (e)-(h) NO and (i)-(l) O_2 on B_xN_y-graphene-Co systems. The isosurface value is 0.002 e/bohr^3.

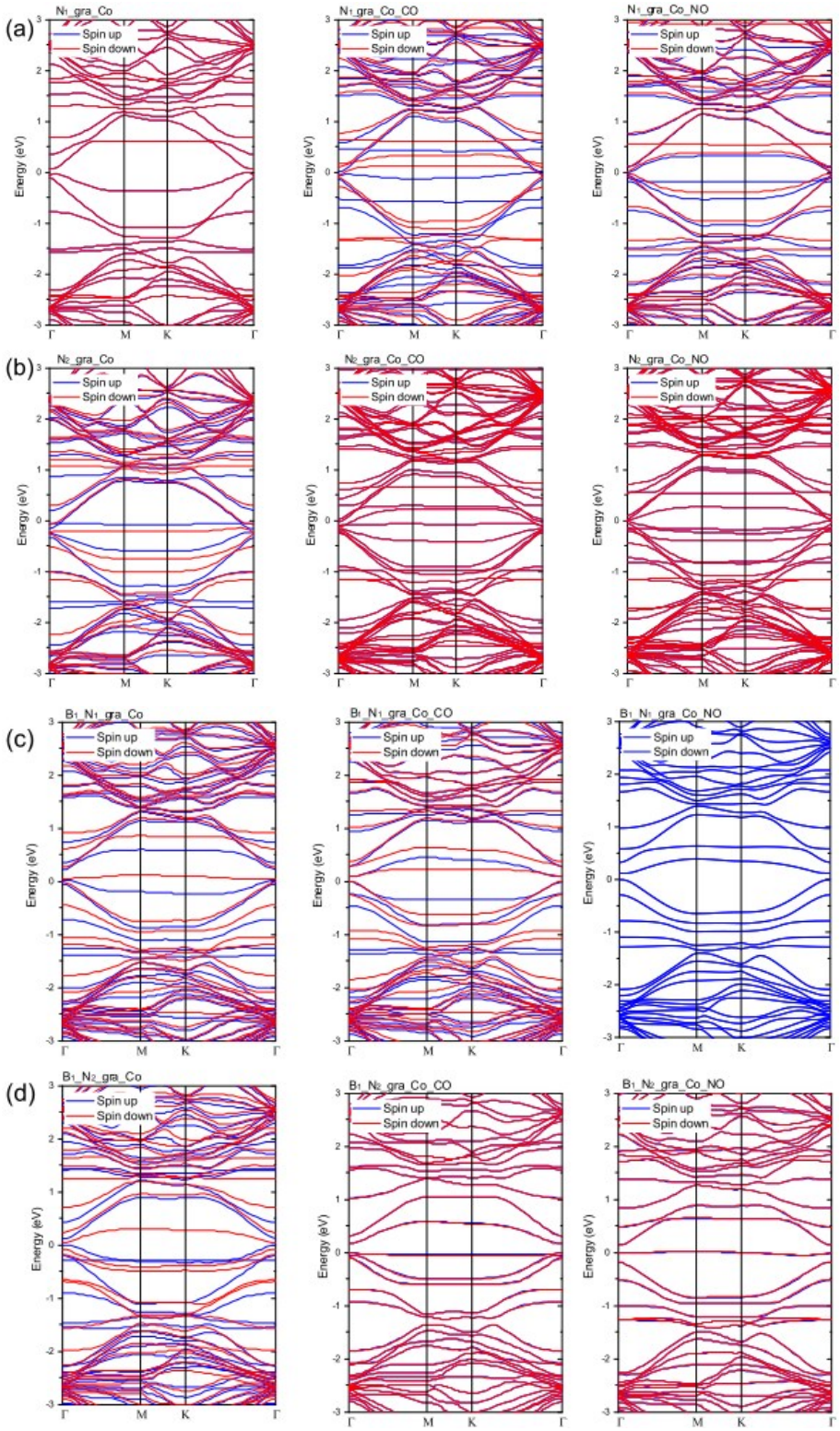

Fig.S6. Varied band structures of (a) N_1-graphene-Co, (b) N_2-graphene-Co, (c) B_1N_1-graphene-Co and (d) B_1N_2-graphene-Co sheets without (or with) CO and NO adsorption.

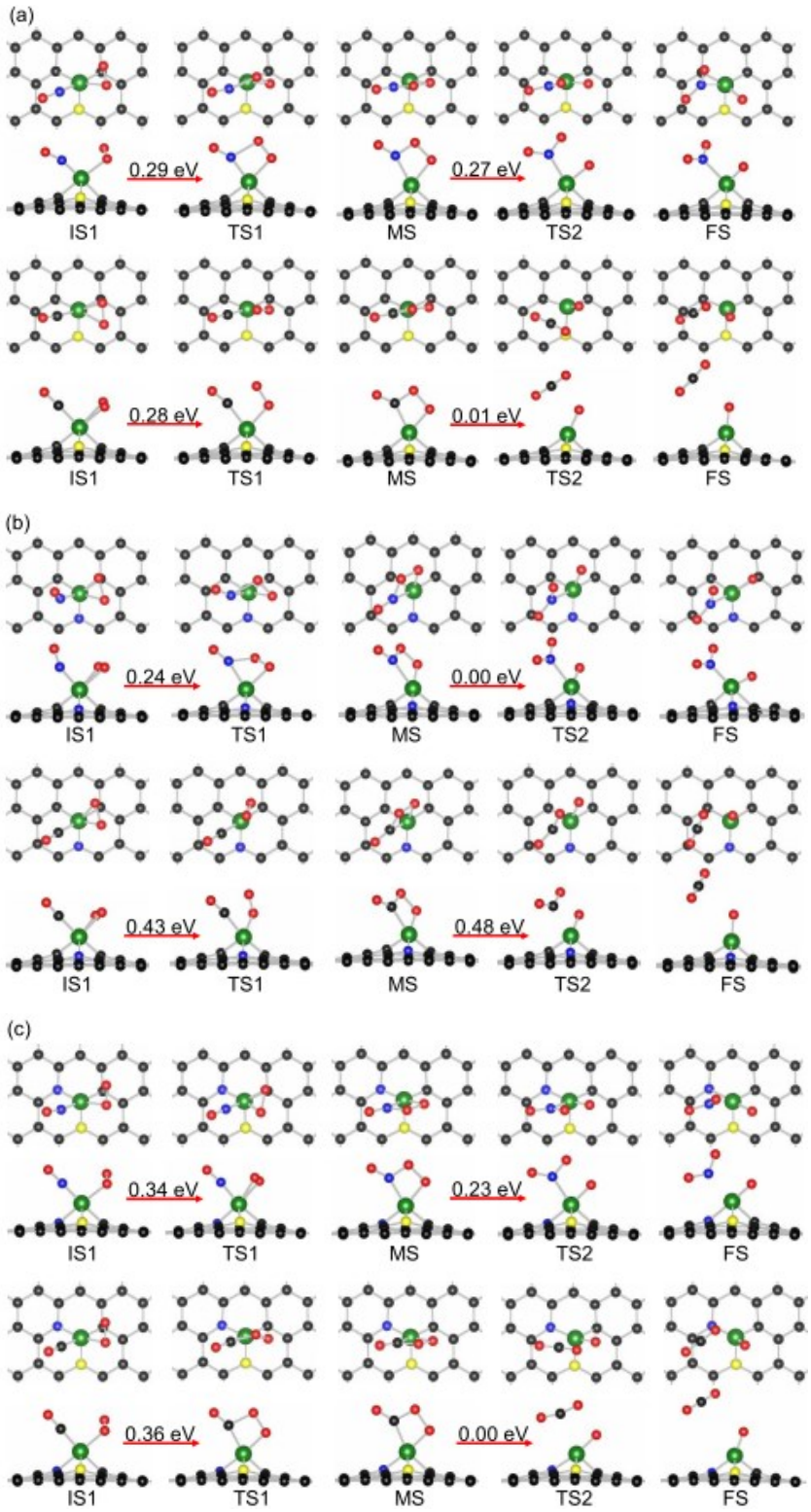

Fig.S7. Catalytic reactions for NO and CO oxidation via LH mechanism on (a) B_1-graphene-Co, (b) N_1-graphene-Co and (c) B_1N_1-graphene-Co sheets. Black, yellow, blue, green and red balls represent C, B, N, Co and O atoms, respectively.