Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table S1. Adsorption energies (E_{ads}) for CO, NO and average E_{ads} for 2CO, 2NO on different graphene-Pt sheets by using the DFT-D2 calculations.

Substrates	DFT-D2			
	CO E_{ads}(eV)	NO E_{ads}(eV)	2CO E_{ads}(eV)	2NO E_{ads}(eV)
1B-gra-Pt	0.97	1.68	0.91	1.35
2B-gra-Pt	1.21	1.39	0.85	1.15
3B-gra-Pt	0.94	1.12	0.69	1.00
1N-gra-Pt	1.30	2.18	1.39	1.47
2N-gra-Pt	2.37	3.05	1.80	1.87
3N-gra-Pt	3.09	4.52	1.97	2.51
1B-1N-gra-Pt	1.68	2.06	0.86	1.44
1B-2N-gra-Pt	2.42	2.98	1.40	1.88
2B-1N-gra-Pt	1.02	1.97	0.88	1.26
SV-gra-Pt	0.28	1.25	0.99	1.39

Table S2. The amounts of transfer charge ($\triangle q$, e) from graphene-Pt substrates to CO, NO, 2CO or 2NO molecules.

Substrates	CO	NO	2CO	2NO
1B-gra-Pt	0.24	0.40	0.21	0.49
2B-gra-Pt	0.14	0.36	0.19	0.40
3B-gra-Pt	0.15	0.36	0.22	0.34
1N-gra-Pt	0.21	0.46	0.26	0.54
2N-gra-Pt	0.24	0.45	0.25	0.55
3N-gra-Pt	0.30	0.47	0.31	0.60
1B-1N-gra-Pt	0.21	0.42	0.20	0.56
1B-2N-gra-Pt	0.24	0.42	0.28	0.62
2B-1N-gra-Pt	0.24	0.36	0.21	0.50
SV-gra-Pt	0.25	0.47	0.27	0.58

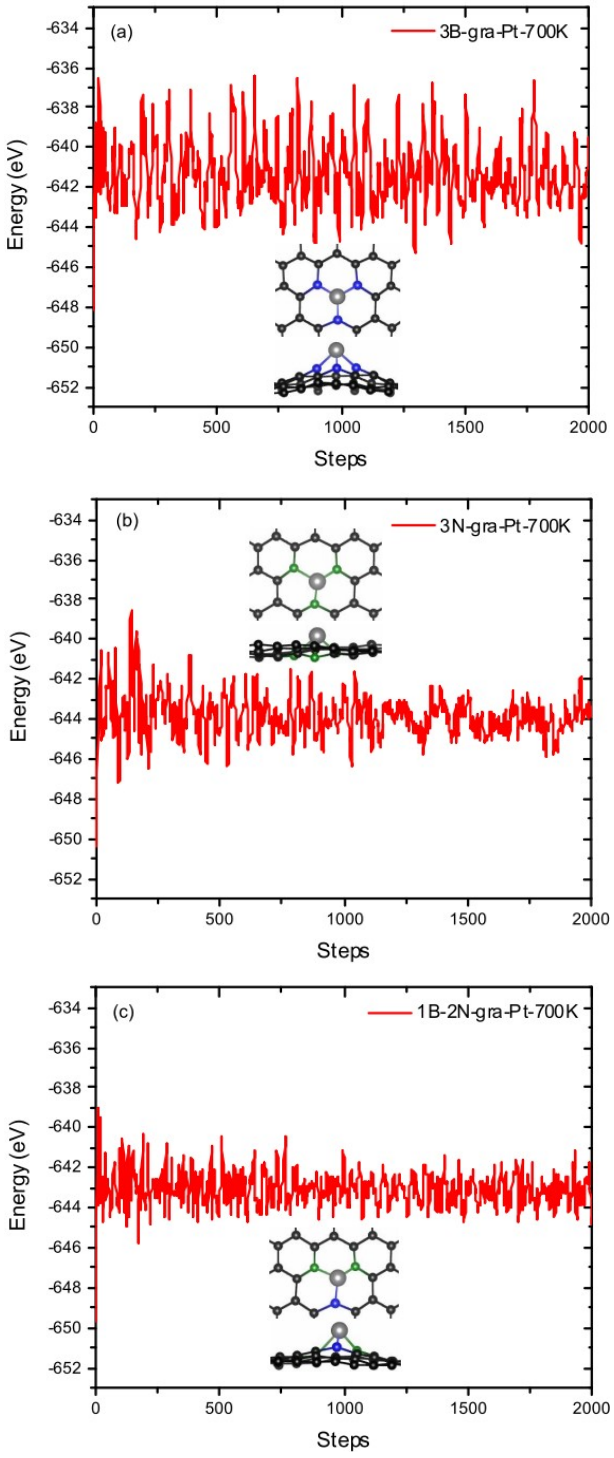

Fig.S1. Stable structures for (a) 3B-graphene-Pt, (b) 3N-graphene-Pt and (c) 1B-2N-graphene-Pt from the molecular dynamics simulation at 700 K.

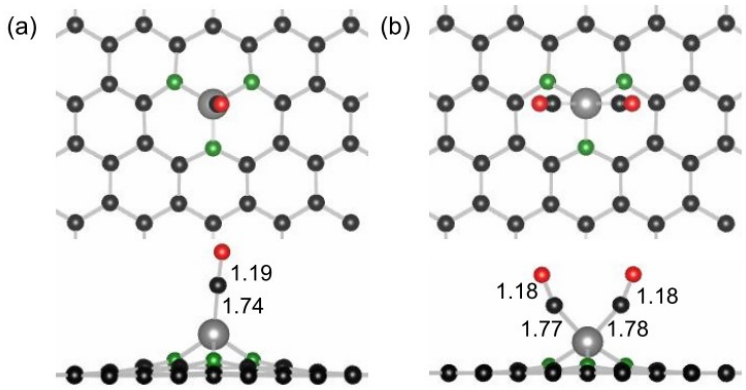

Fig.S2. Initial adsorption sites for (a) CO and (b) 2CO molecules anchored at 3N-graphene-Pt sheet.