

## Supporting Information

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Here, we make a detailed comparisons between calculated results with general gradient approximation (GGA)<sup>1</sup> and local density approximation (LDA)<sup>2</sup>, remaining the same other parameters.

Table S1 lists the binding energies of metals on GO in LDA and GGA with spin polarization, respectively. It could be found out that LDA will some overestimate the binding energies comparing with GGA in most cases. However, the tendency of results in LDA and GGA are very similar. Li and Al could be anchored stably by hydroxyl and epoxy groups on GO, and Li@GO-ADE, Al@GO-ADE are also the most stable configurations for each metal decorated graphene oxide.

**Table S1** Binding energies of different metals on GO in LDA and GGA with spin polarization.

(Units: eV)

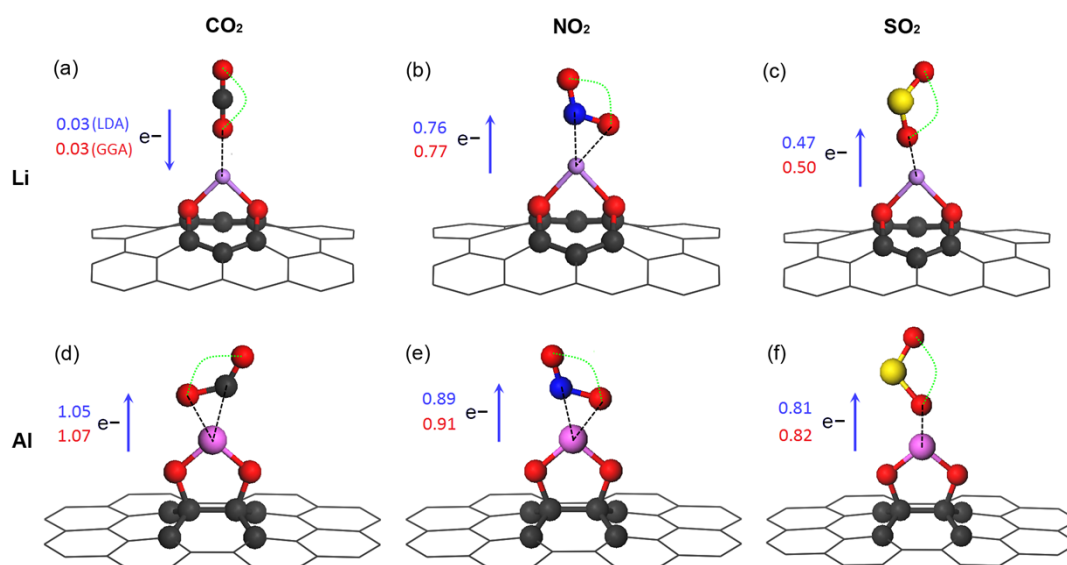
Groups	ADE		CDE		ADH		CDH	
	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA
Li	-3.55	-3.45	-2.39	-2.15	-1.19	-1.26	-0.83	-0.98
Al	-5.72	-5.40	-2.13	-1.74	-3.32	-3.14	-3.12	-2.90

Besides, table S2 shows that LDA and GGA give the same tendency in gas binding energies on decorated GO, despite there are some differences of the specific values for each gas. The main conclusions are also remained. Li decorated GO has an outstanding adsorption ability of acidic gases as well as a relatively weak interaction with O<sub>2</sub>. Al decorated GO displays much higher binding energy of all acidic gases.

**Table S2** Binding energies of gases on metal decorated GO in LDA and GGA with spin polarization. (Units: eV)

GASES	O <sub>2</sub>		CO <sub>2</sub>		NO <sub>2</sub>		SO <sub>2</sub>	
	LDA	GGA	LDA	GGA	LDA	GGA	LDA	GGA
<b>Li@GO-ADE</b>	-0.49	-0.67	-0.31	-0.27	-1.25	-0.88	-0.48	-0.45
<b>Li@GO-CDE</b>	-1.62	-2.00	-0.48	-0.46	-2.20	-2.20	-1.42	-1.51
<b>Al@GO-ADE</b>	-3.57	-3.49	-0.91	-0.57	-3.60	-3.13	-2.15	-1.91
<b>Al@GO-ADH</b>	-8.07	-7.71	-0.19	-0.02	-3.12	-1.95	-0.44	-0.25

Furthermore, from Fig S1, the electron transfers between acidic gases and metal decorated GO are almost the same in LDA and GGA cases.



**Fig S1** The electrons transfers between acidic gases (a, d are CO<sub>2</sub>; b, e are NO<sub>2</sub>; c, f are SO<sub>2</sub>) and metal decorated GO (a~c are Li decorations; d~f are Al decorations) in LDA and GGA with spin polarization.

The calculated binding energies with GGA are quantitatively lower than that with LDA, while the qualitative rules are similar. It can be found that the physics is not modified for different functions.

## Reference

1. J. P. Perdew, K. Burke, M. Ernzerhof. *Phys. Rev. Lett.* 1996, **77**, 3865.
2. W. Kohn, L. Sham. *J. Phys. Rev.*, 1965, **137**, A1697–A1705.