Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Interfacial Interaction of Ag Nanoparticles with Graphene Oxide supports for Improving NH_3 and NO Adsorption: a First-Principles Study

Supporting Information

Shaobin Tang, [*,†] Weihua Wu, [†] and Jianping Yu[*,‡]

[†]Key Laboratory of Organo-Pharmaceutical Chemistry of Jiangxi Province, Gannan Normal University, Ganzhou 341000, China

[‡]School of life and environmental sciences, Gannan Normal University, Ganzhou 341000, China

E-mail address: tsb1980@xmu.edu.cn, yujianping402871@sina.com

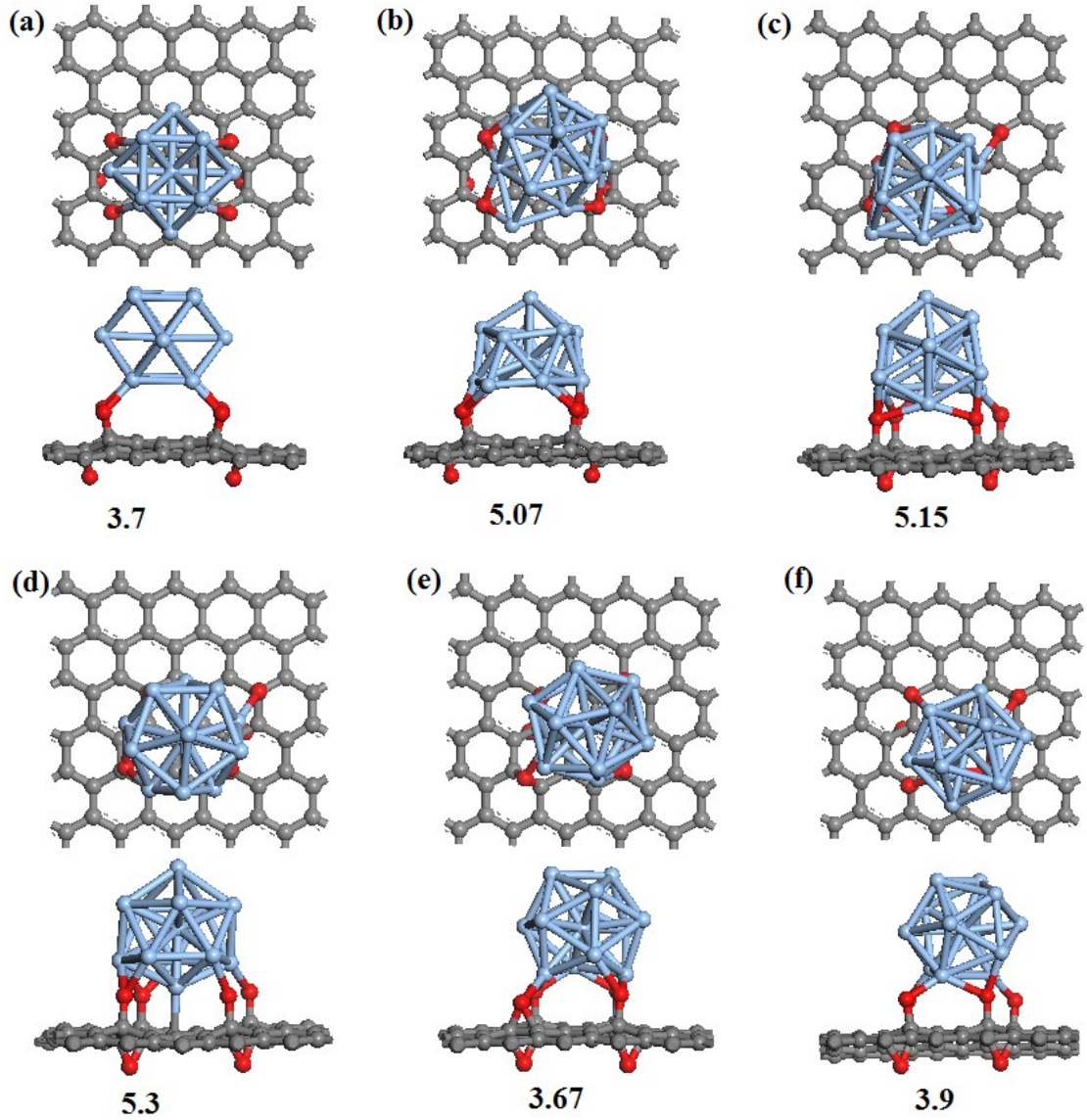

Figure S1. Top and side views of optimized structures and corresponding binding energies (in eV) for Ag_{13}/GOs with different direction of NPs relative to graphene surface: Ag_{13} with initial (a)-(c) cuboctahedron and (d)-(f) icosahedron structures.

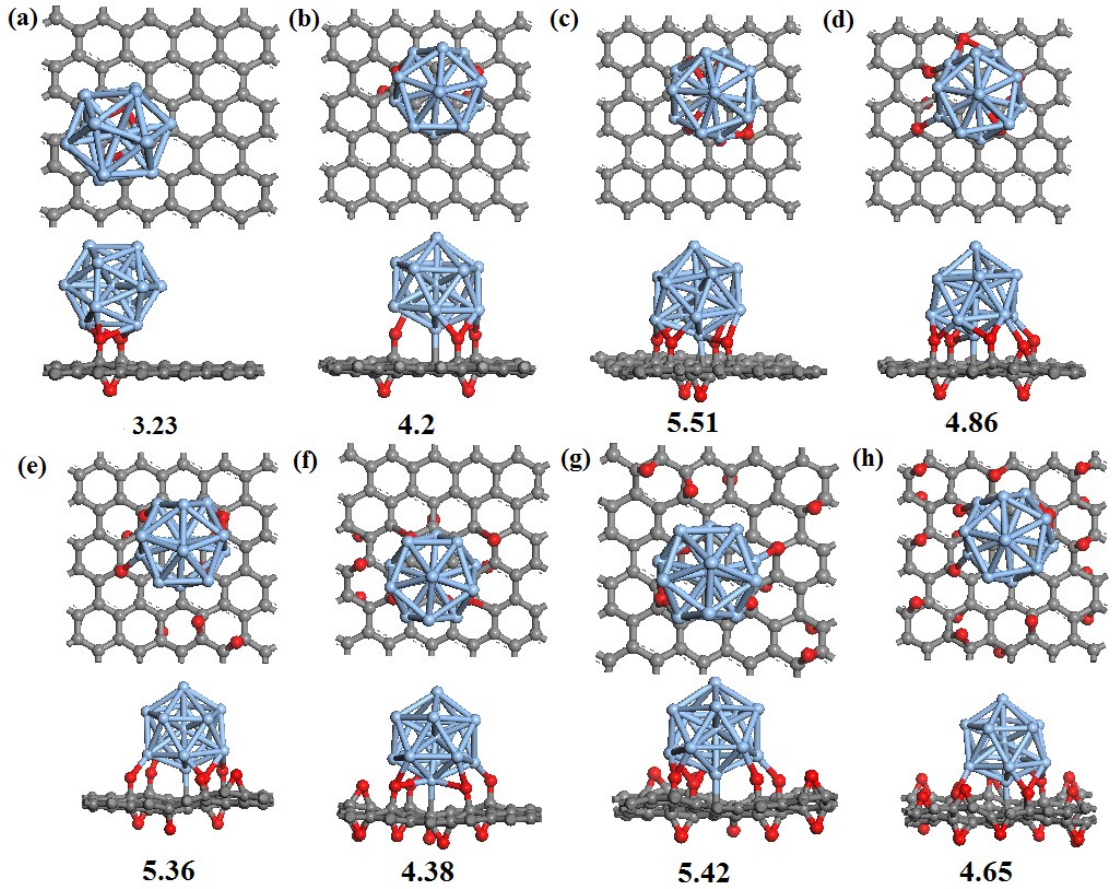

Figure S2. Top and side views of optimized structures and corresponding binding energies (in eV) for Ag_{13}/GOs with different oxidation level. (a) GO-3O, (b) GO-5O, (c) GO-6O-2, (d) GO-7O, (e) GO-9O, (f) GO-12O, and (h) GO-20O.

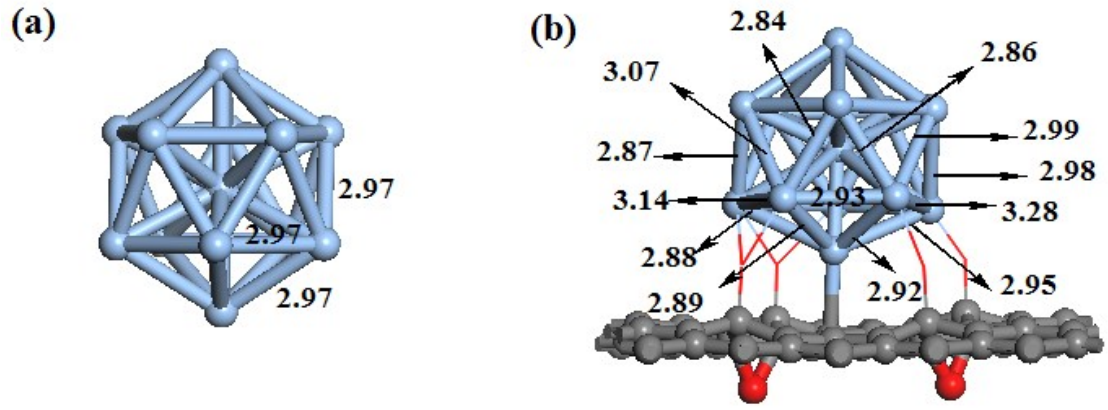

Figure S3. The changes in Ag–Ag bond length (in Å) of Ag_{13} after deposition on GO-6O-1. The Ag–O and O–C bonds are shown with red solid line.

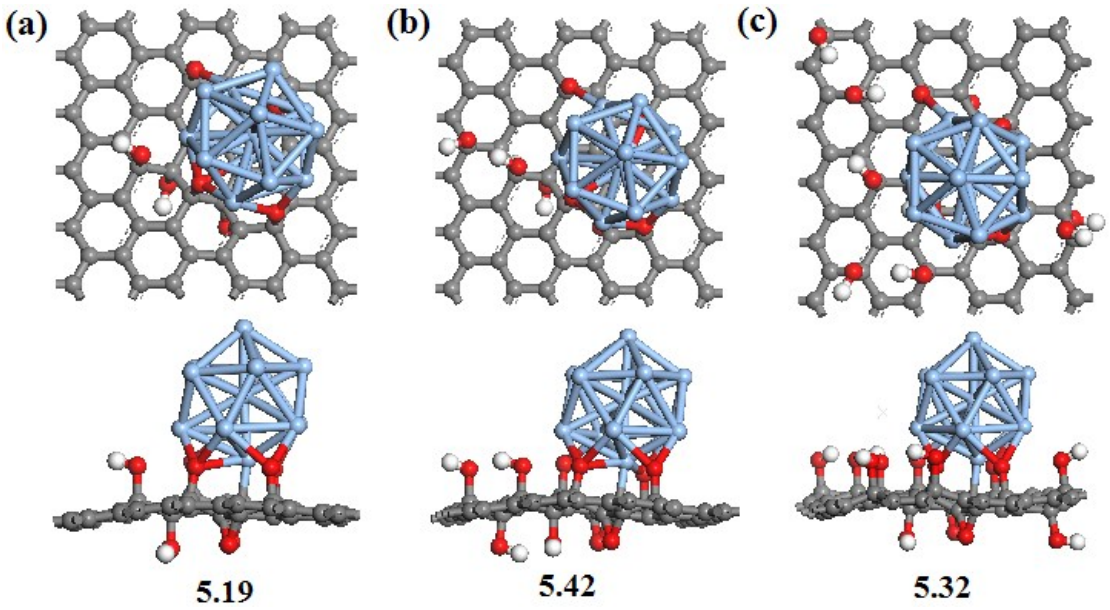

Figure S4. Top and side views of optimized structures and corresponding binding energies (in eV) for Ag_{13} deposited on GO-6O-1 with additional hydroxyl groups. (a) 2, (b) 4, and (c) 8 OH groups.

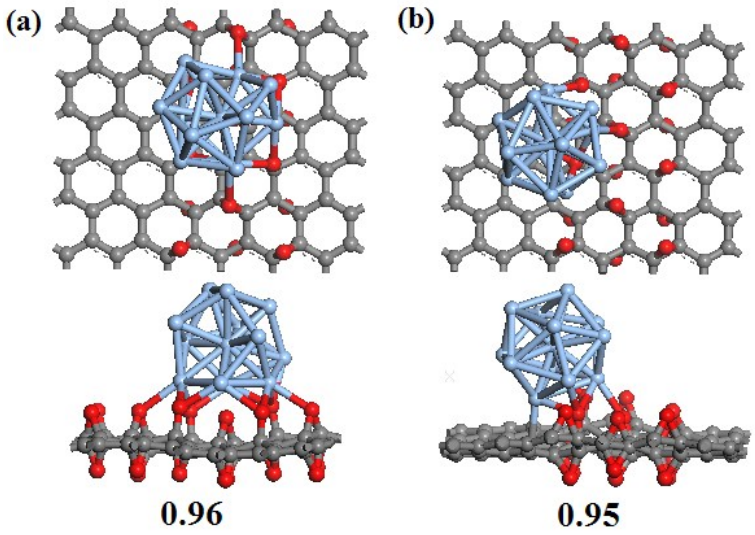

Figure S5. Top and side views of optimized structures and corresponding binding energies (in eV) for Ag_{13}/GO3 with two binding models.

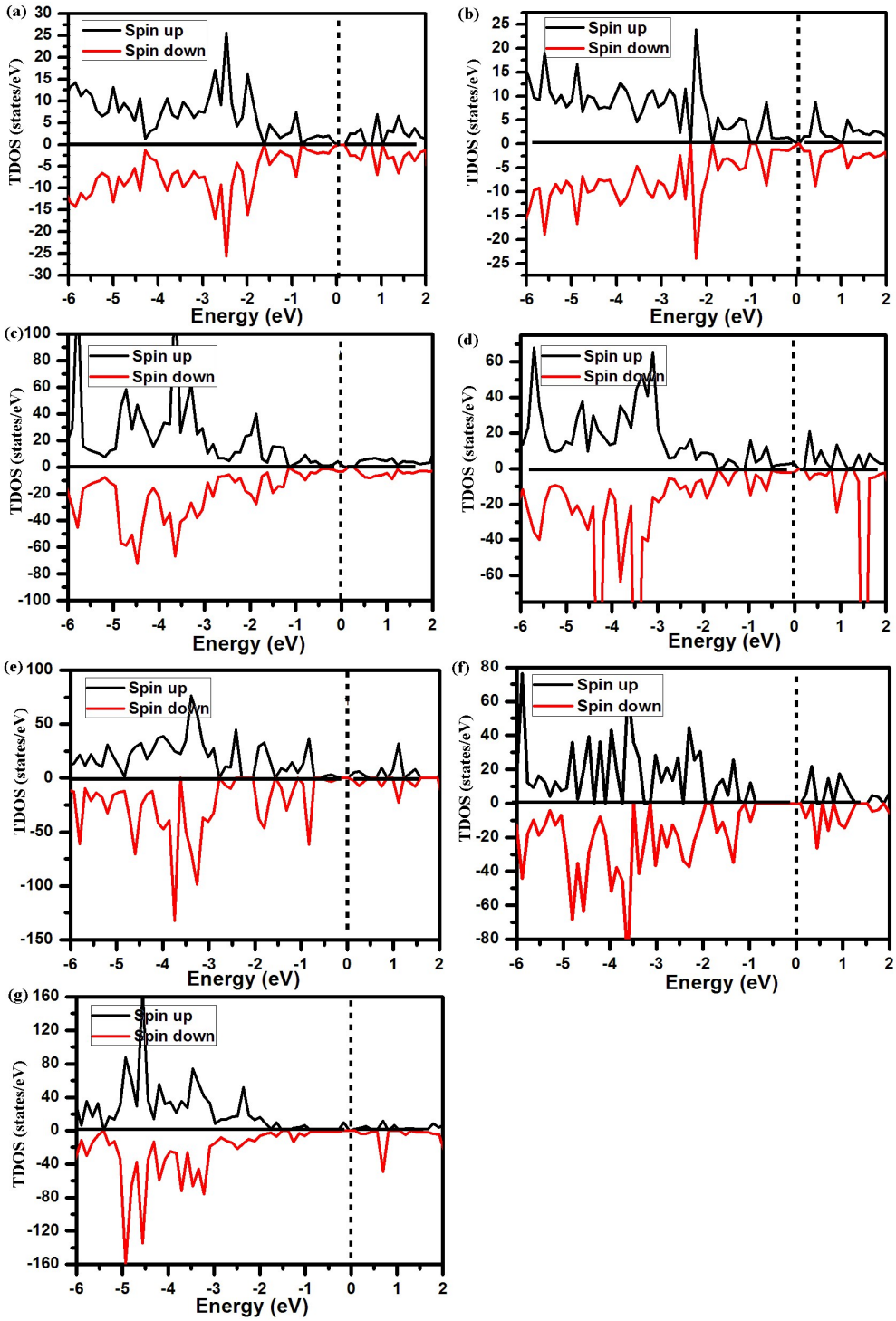

Figure S6. The spin-polarized TDOS of GOs and Ag_{13}-GOs hybrid with different oxygen concentration. (a) GO-6O-1, (b) GO-6O-2, (c) Ag_{13}/GO-6O-1, (d) Ag_{13}/GO-6O-2, (e) Ag_{13}/GO-14O-1, (f) Ag_{13}/GO-17O, and (g) Ag_{13}/GO2. The Fermi level is set to 0.

Table S1. Summary of calculated results for NH_3 and NO adsorptions on selected GOs models: the adsorption energy (E_{ad}), the distance between adsorbate and binding site of GOs (d), and the charge transfers from the molecule to GOs (ΔQ).

substrate	adsorbate	binding site*	E_{ad} (eV)	d (Å)	ΔQ (e)
GO-6O-1	NH_3	O	-0.13	2.49	0.04
	NO	No	-0.15	2.61	0.17
GO-14O-1	NH_3	O	-0.18	2.43	0.06
GO-5O-2OH	NH_3	H from OH	-0.56	1.76	0.09
	NH_3	O from OH	-0.15	2.33	0.01
	NO	H from OH	-0.12	2.51	0.12

* Selected geometrical structures are shown in Figure S7.

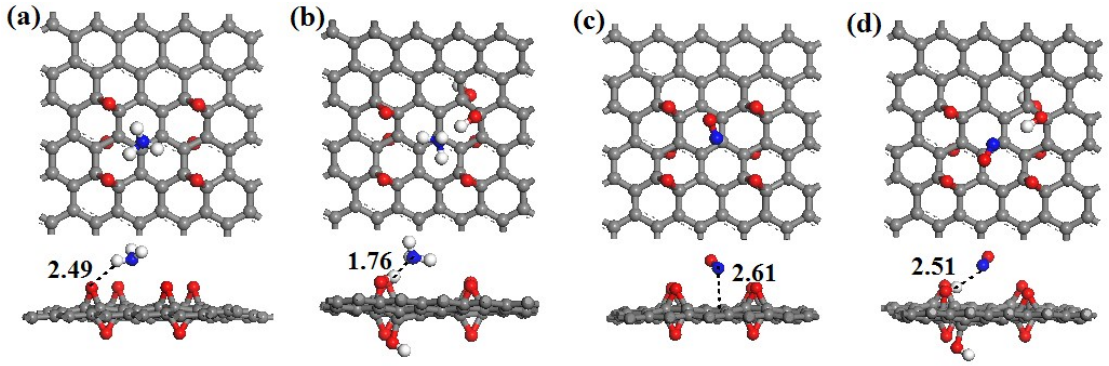

Figure S7. Top and side view of geometrical structures (distance in Å) for adsorption of NH3 and NO on pristine GOs. (a, c) GO-6O-1 and (b, d) GO-5O-2OH.

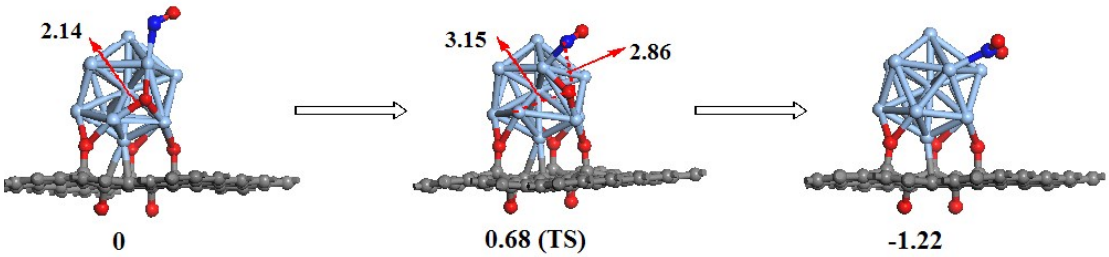

Figure S8. The geometrical structures (distance in Å) of initial state, transition state (TS), and final state for oxidation of adsorbed NO to NO_2 on $Ag_{13}O$/GO-5O. All energies (in eV) are relative to initial state.

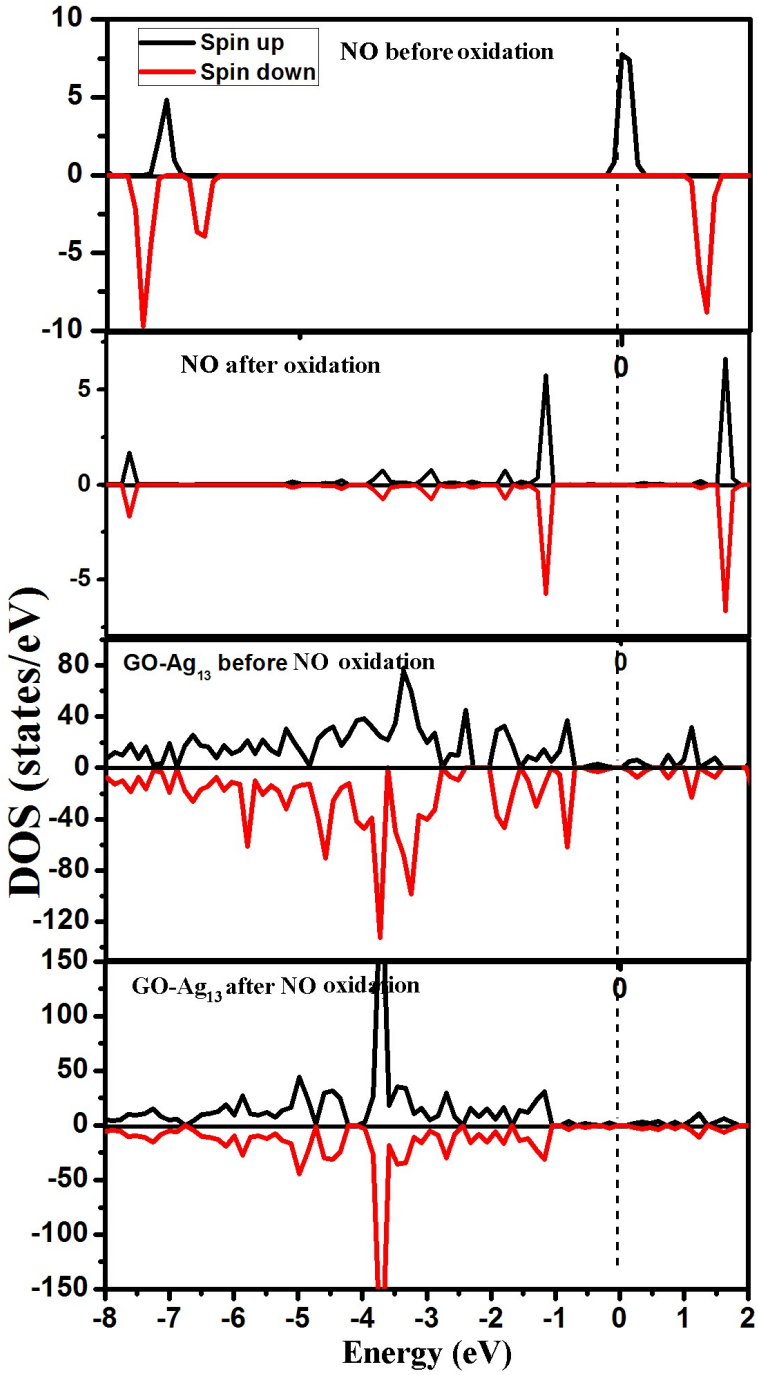

Figure S9. The spin-polarized TDOS and PDOS of NO and Ag_{13}/GO-14O-1 before and after NO oxidation on hybrid. The Fermi level is set 0.