Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Structural and electronic properties of Pd-decorated graphene oxides and their effects on the adsorption of nitrogen oxides: insights from density functional calculations

Shaobin Tang* and Jiayi Zhu

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

* *E-mail address:* tsb1980@xmu.edu.cn

Table S1: Summary of calculated results for the adsorption of Pd on rGOs with both hydroxyl and epoxy groups: the binding energy (E_b), the distance between Pd and its neighboring C (d_1), and O (d_2) atoms.

Structure	binding site	E_b (eV)	d_1 (Å)	d_2 (Å)
Pd@G-O-OH-1a	C	1.45	2.12	2.42
Pd@G-O-OH-1b	C and O	2.25	2.13	2.06
Pd@G-O-OH-2a	C	1.06	2.25	
Pd@G-O-OH-2b	C and O	1.36	2.13	2.07
Pd@G-O-OH-2c	O	0.08	2	
Pd@G-2O-OH-1a	C	1.63	2.1	2.69
Pd@G-2O-OH-1b	O	2.25		2.04 (2.3)
Pd@G-2O-OH-1c	O	2.66		1.97
Pd@G-2O-OH-1d	O	2.58		1.96
Pd@G-2O-OH-2	C and O	1.78	2.08	2.05

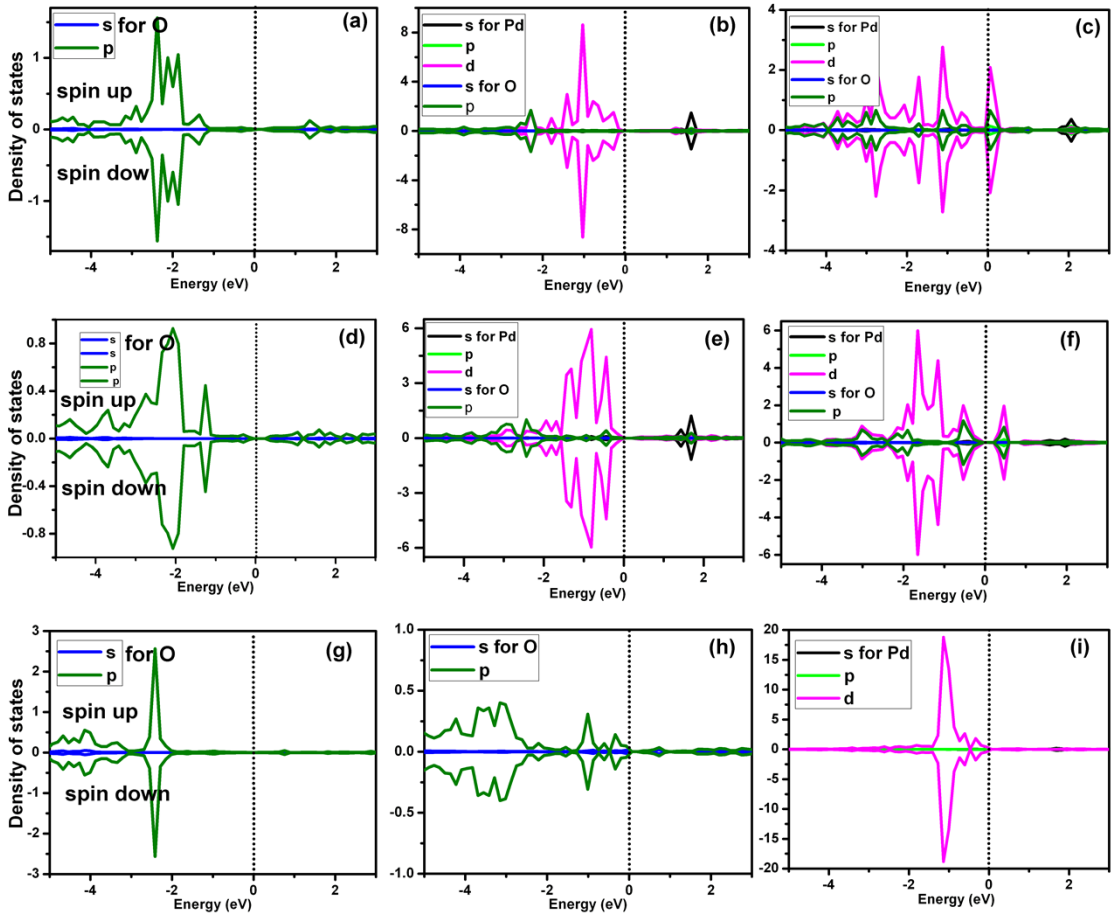

Figure S1. The spin-polarized Projected density of states (PDOS) of O atom from GO before and after Pd interaction and the PDOS of adsorbed Pd for Pd-decorated GOs. (a) G-2O-1, (b) Pd@G-2O-1a, (c) Pd@G-2O-1c, (d) G-2O-2, (e) Pd@G-2O-2a, (f)

Pd@G-2O-2b, (g) G-2OH-2, and (h)-(i) Pd@G-2OH-2. The Fermi level is set to 0.

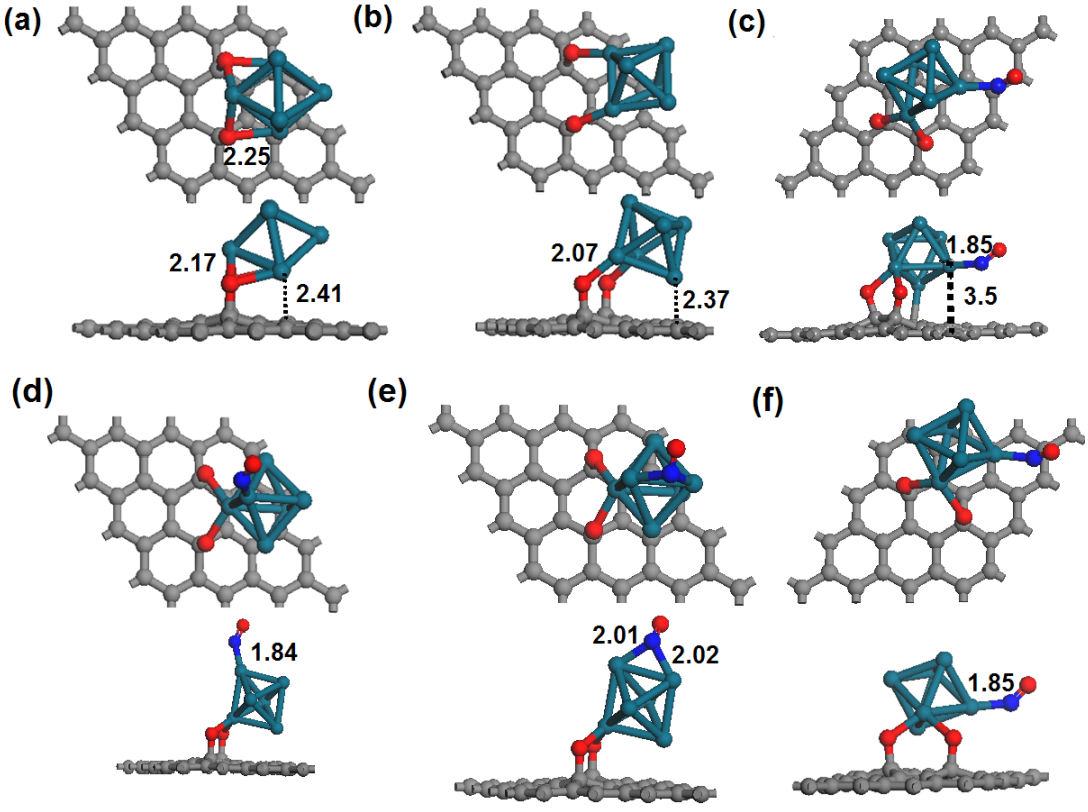

Figure S2. Top and side views of optimized structure (distance in Å) for Pd_6 deposited on G-2O-1 (a)-(b) and NO adsorbed on Pd_6-rGO hybrid (e)-(h). (a) Pd_6@ G-2O-1-c and (b) Pd_6@G-2O-1-d. Adsorption of NO at (c) Pd**5** site of Pd_6@ G-2O-1-a and (d)-(f) various Pd sites of Pd_6@ G-2O-1-b.

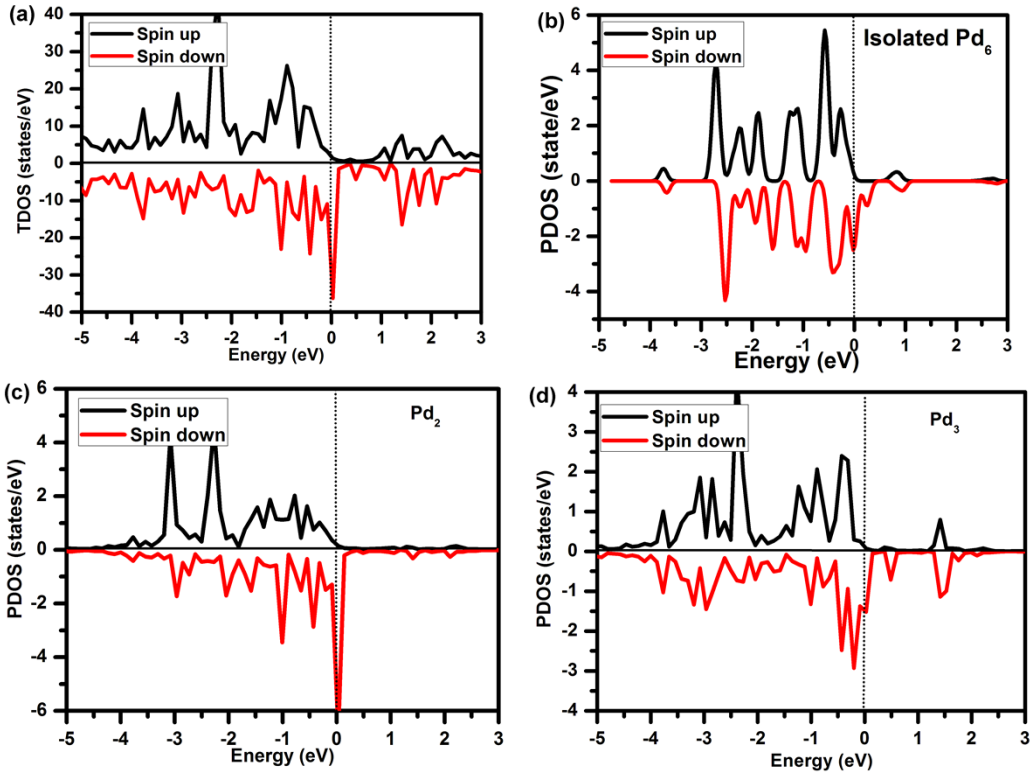

Figure S3. The spin-polarized TDOS and PDOS of Pd atom for isolated Pd_6 cluster and Pd cluster adsorbed rGO. (a) Pd_6@ G-2O-1-a and (b) one Pd atom, (c) Pd**2** and (d) Pd**3** of Pd_6@ G-2O-1-a. The Fermi level is set to 0.