Double-platelet Pd@ZnO microcrystals for NO_2 chemical sensors: a facile synthesis and DFT investigation

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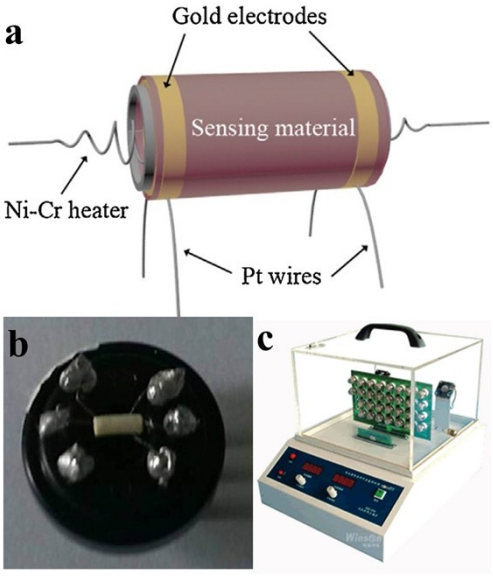

Fig. S1 (a) The structural illustration, (b) photo of an ZnO sensor and (c) measurement setup.

material	(hkl)	I/I_0	TC [%]
D-ZnO	(100)	7.73	33.3
	(002)	7.55	32.5
	(101)	7.96	34.2
S-ZnO	(100)	4.98	38.7
	(002)	3.84	29.9
	(101)	4.03	31.4
Sp-ZnO	(100)	5.14	45.3
	(002)	2.6	22.9
	(101)	3.61	31.8

Table S1. The X-ray diffraction data results of D-ZnO, S-ZnO, and Sp-ZnO.

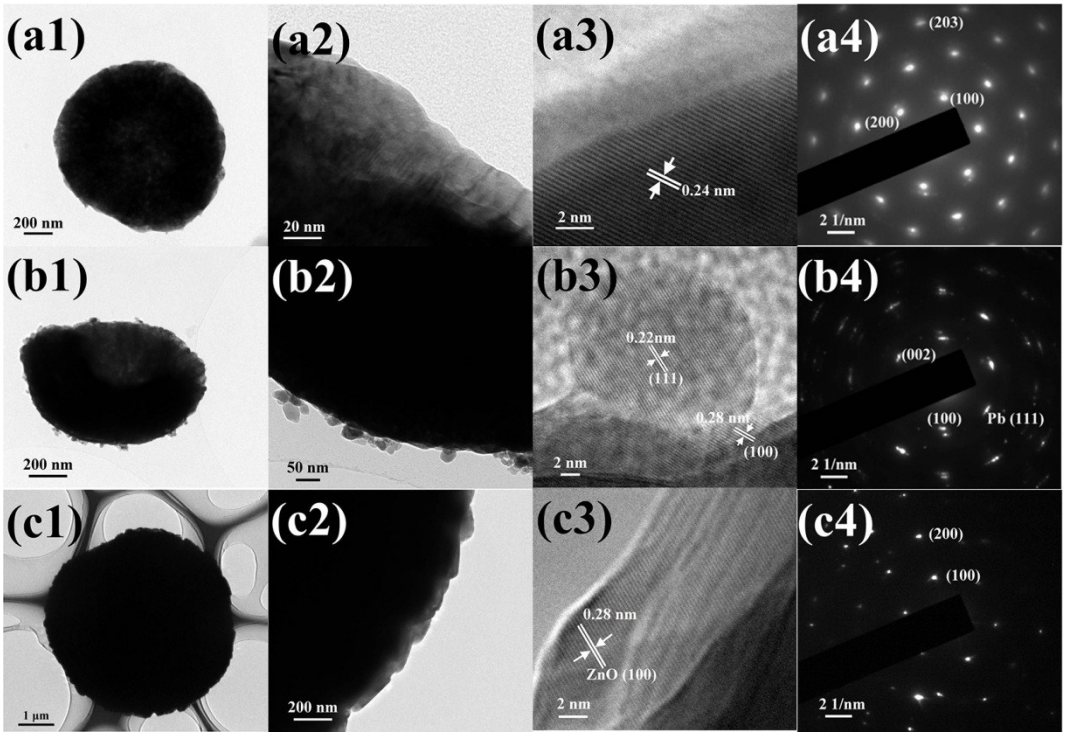

Fig. S2. The TEM, HRTEM and SAED images of S-ZnO (a1-4), S-ZnO-0.05 (b1-4) and Sp-ZnO (c1-4).

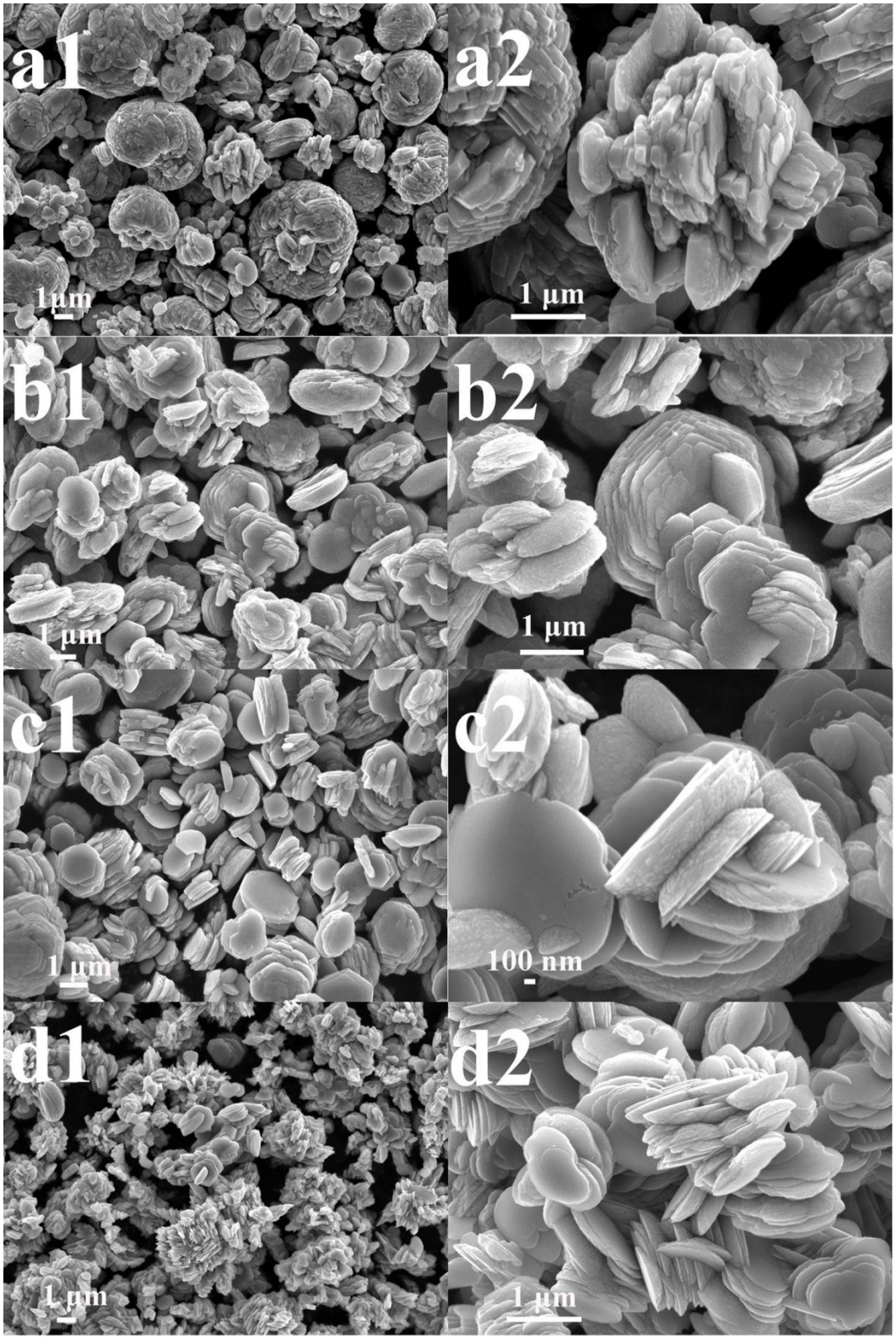

Fig. S3 The SEM of ZnO microcrystals with different amount of sodium citrate: (a1-2) 0.1 mmol; (b1-2) 0.5mmol; (c1-2) 0.8 mmol and (d1-2) 1 mmol.

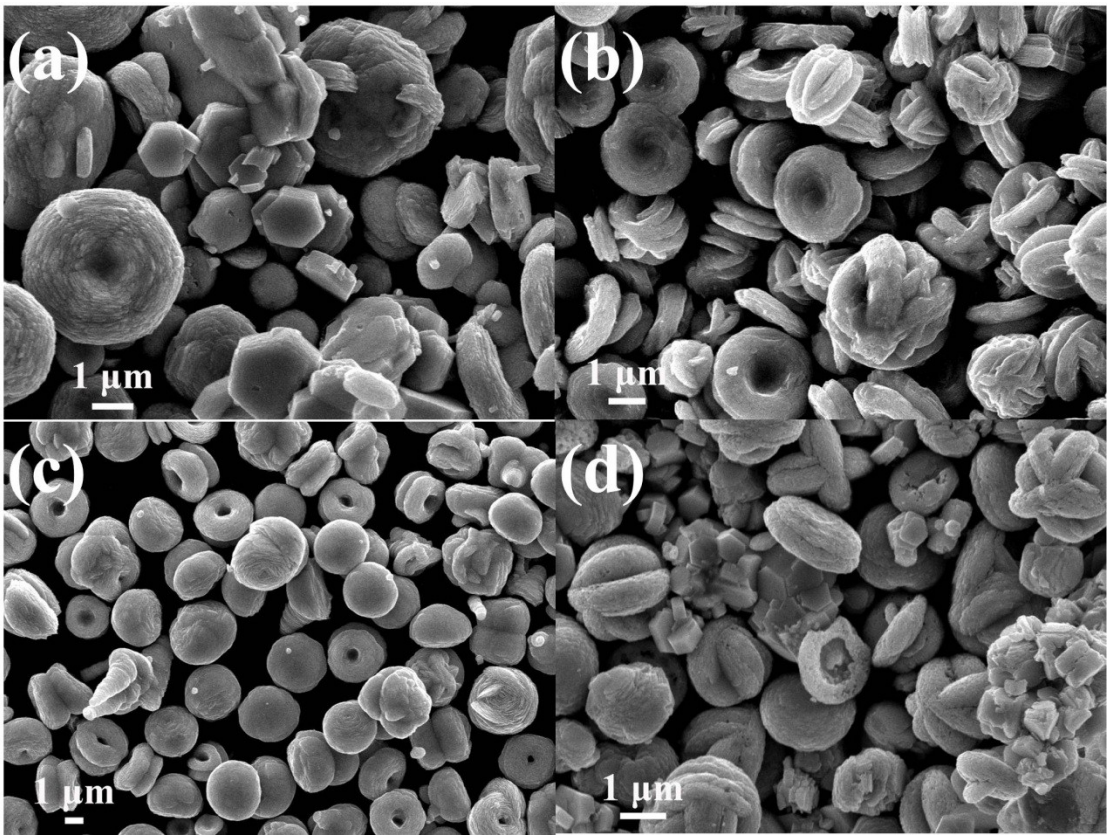

Fig. S4 The SEM of ZnO microcrystals with different the ratio of n-butanol to water: (a) 1:10; (b) 1:5; (c) 1:3 and (d) 1:1

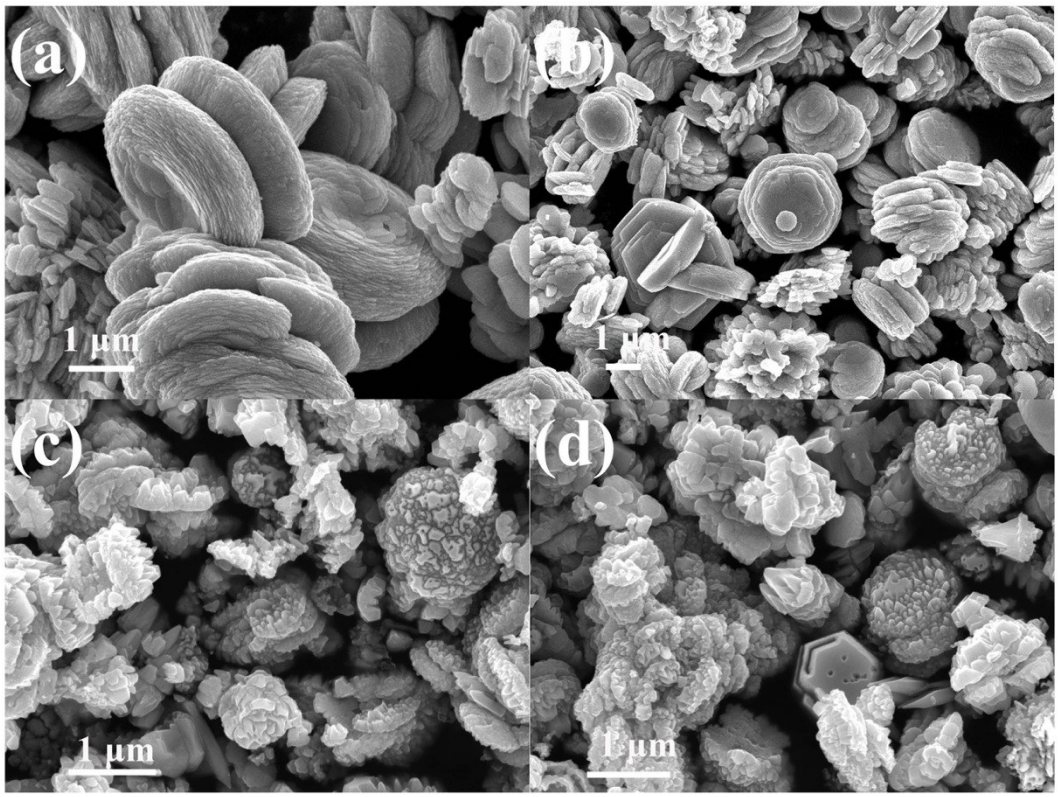

Fig. S5 The SEM of D-ZnO microcrystals at different reaction temperature: (a) 140 ˚C; (b) 160˚C; (c) 180˚C; and (d) 200˚C.

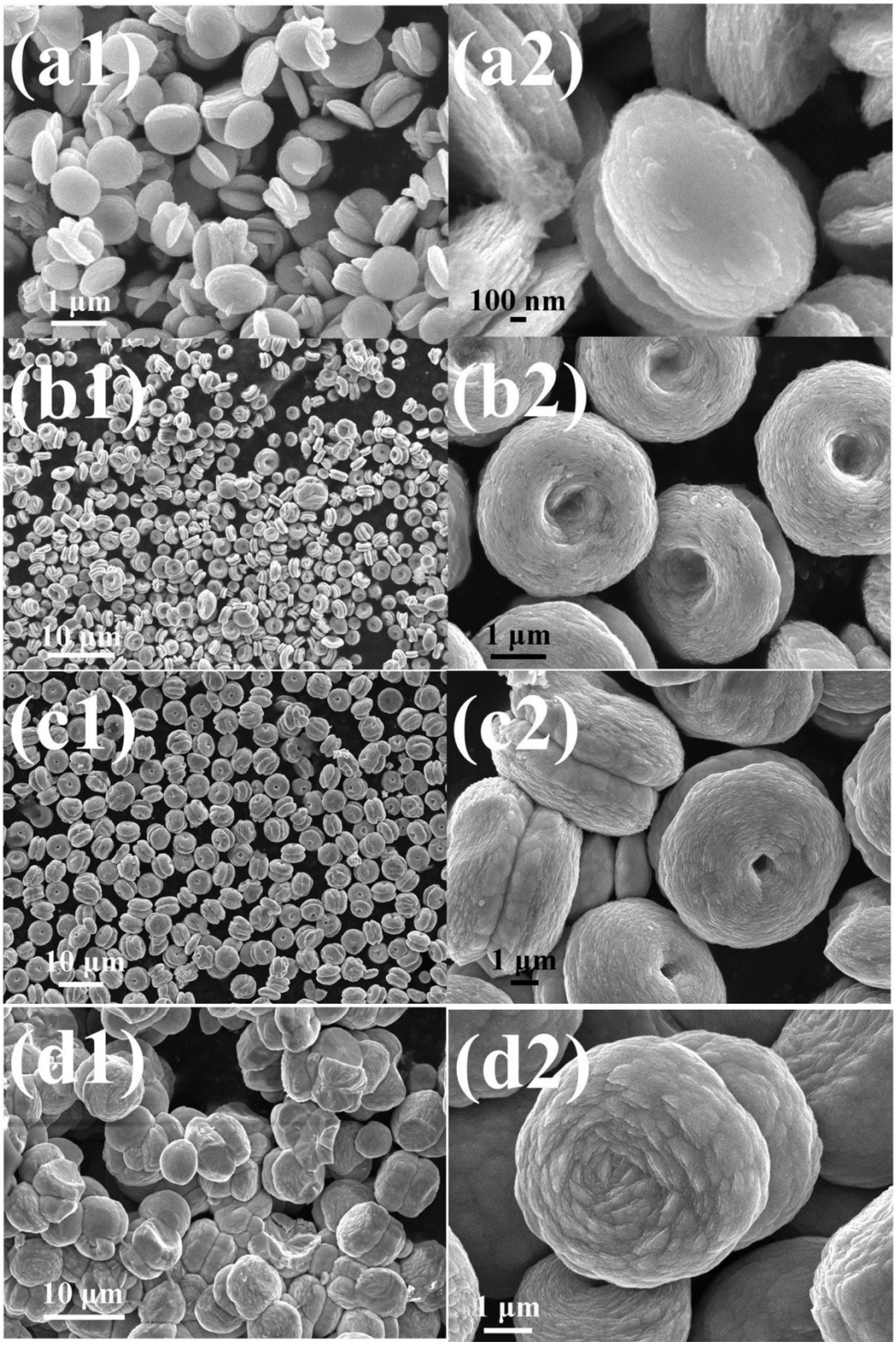

Fig. S6 The SEM of D-ZnO microcrystals at different reaction time: (a) 6h; (b) 15h; (c) 18h; and (d) 24h.

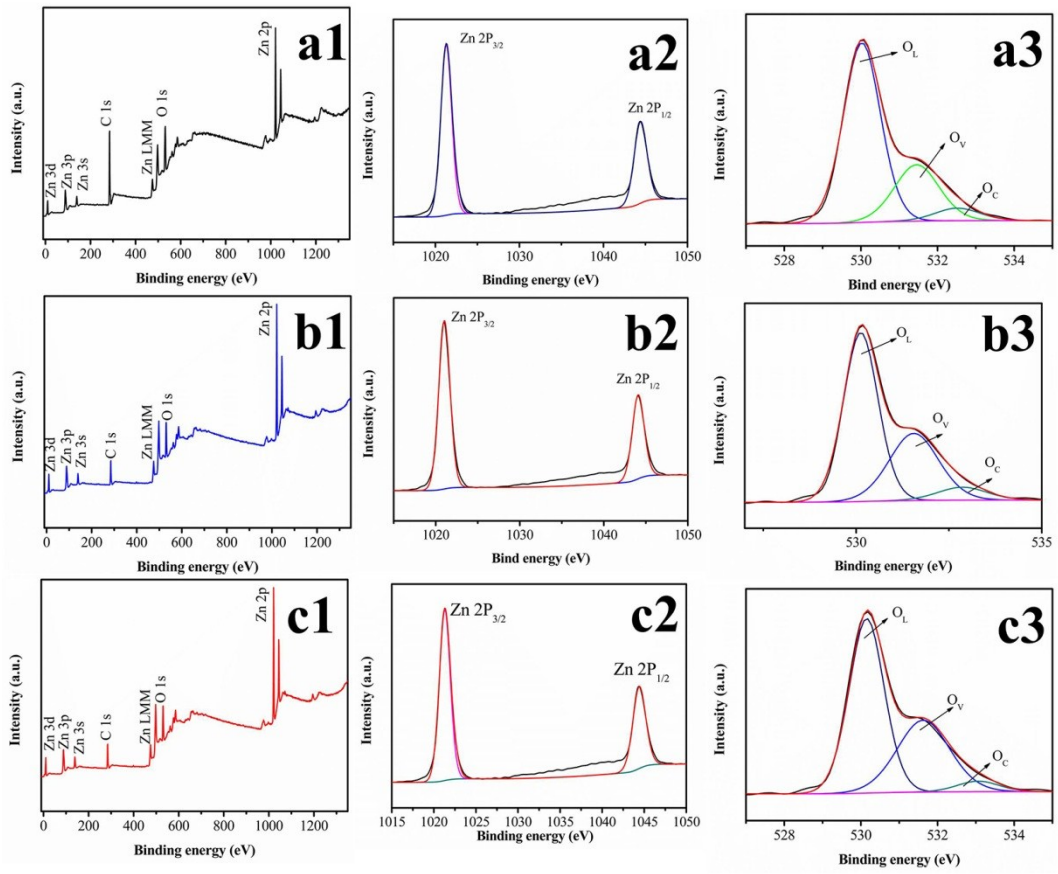

Fig. S7 The XPS spectra of Sp-ZnO (a1-3), S-ZnO (b1-3) and D-ZnO-0.01(c1-3).

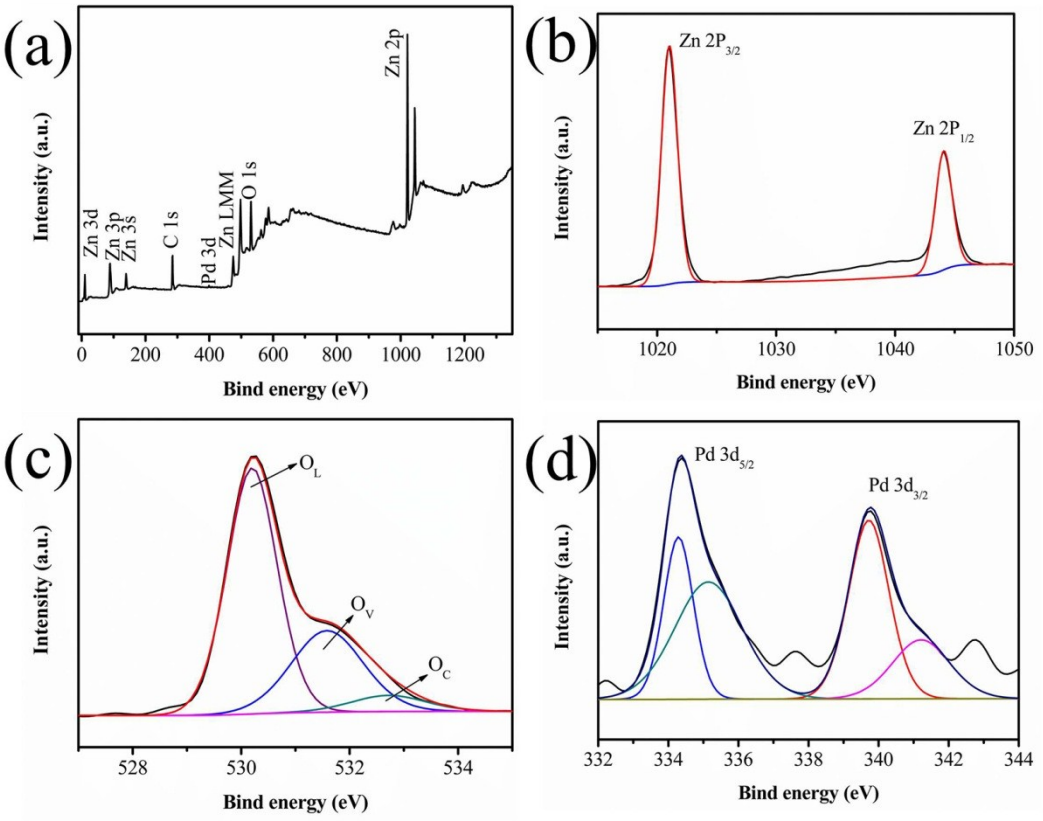

Fig. S8 The XPS spectra of D-ZnO-0.1: (a) full spectrum; (b) Zn 2p; (c) O 1 s; (d) Pd 3d.

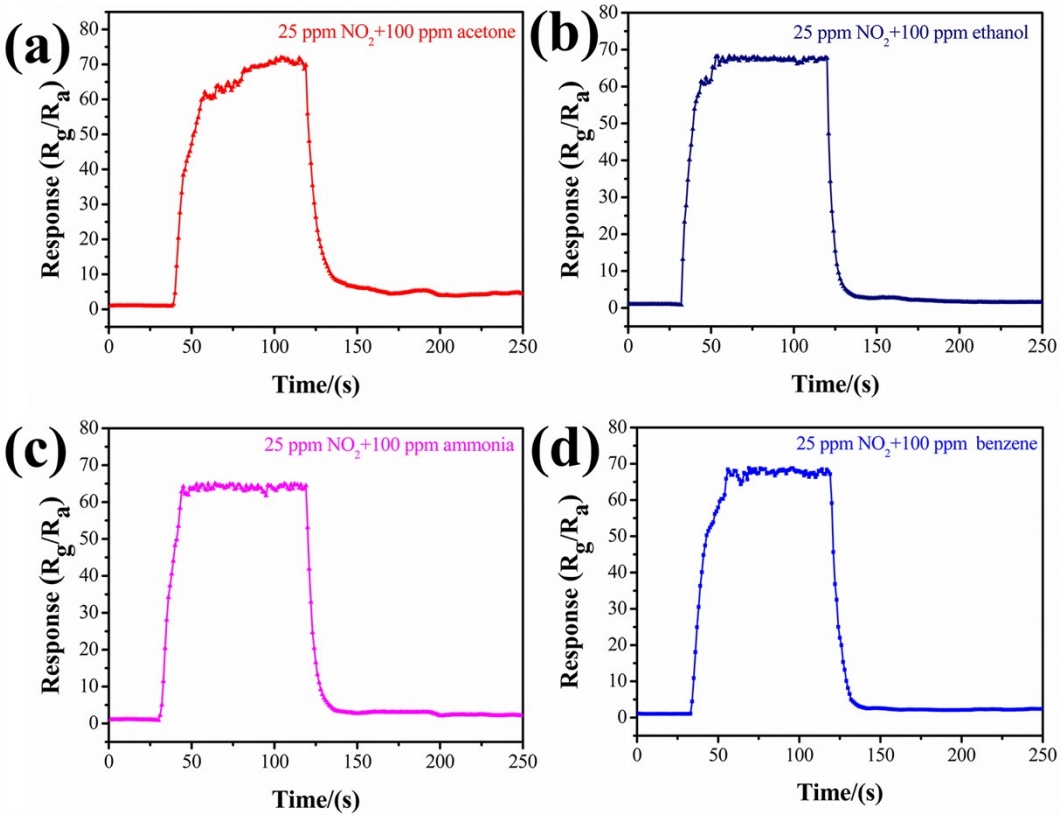

Fig. S9 The dynamic responses of acetone (a), ethanol (b), ammonia (c) and benzene (d) (200 °C 100 ppm) with 25 ppm NO_2, respectively.

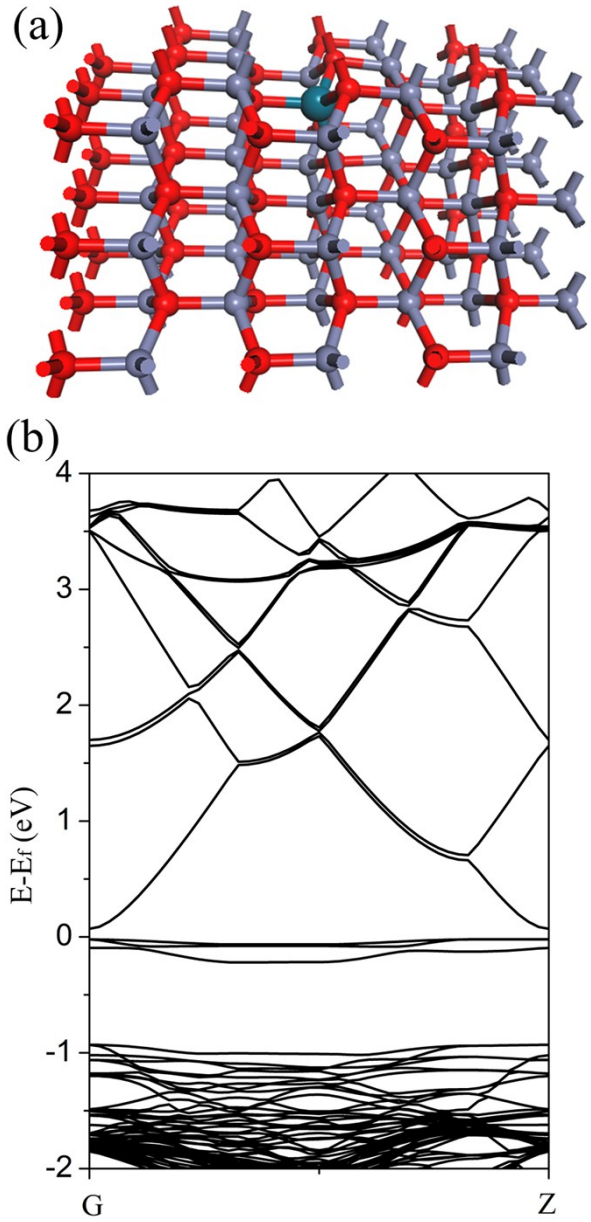

Fig. S10 (a) The favorable configuration Pd-doped ZnO; (b) the band structure of Pd-doped ZnO system. The Fermi level was set to be 0 eV.

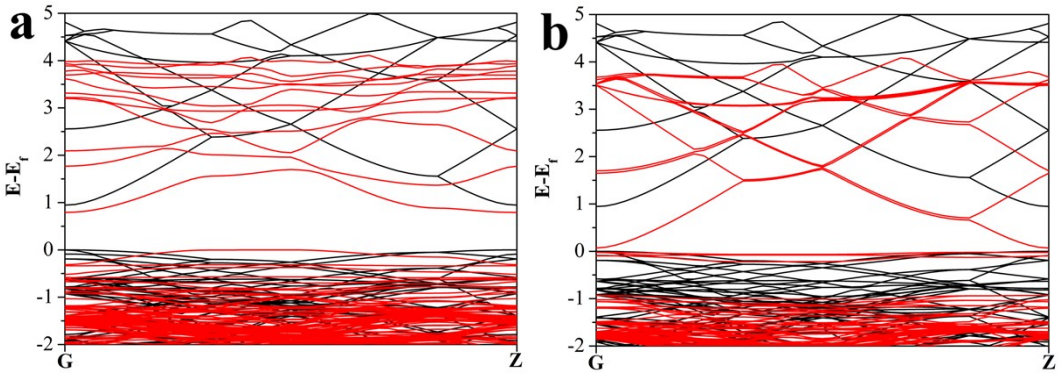

Fig. S11 The band structure of pure supercell ZnO (black line) and Pd-adsorbed oxygen vacancy ZnO (red line) (a), pure supercell ZnO (black line) and Pd-doped ZnO (red line) (b).

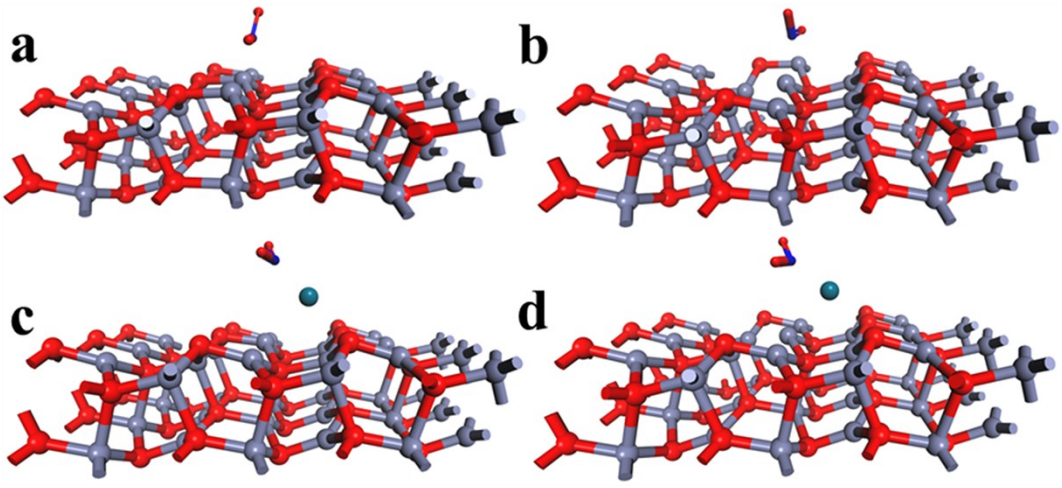

Fig. S12 The favorable configurations of NO_2 adsorption on pristine ZnO (a), Ov-ZnO (b), Pd-ZnO (c), and Ov-Pd-ZnO (d).