Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Material

Promotional Effect of TiO_2 (001) Facet in the Selective Catalytic Reduction of NO with NH_3: In Situ DRIFTS and DFT Studies

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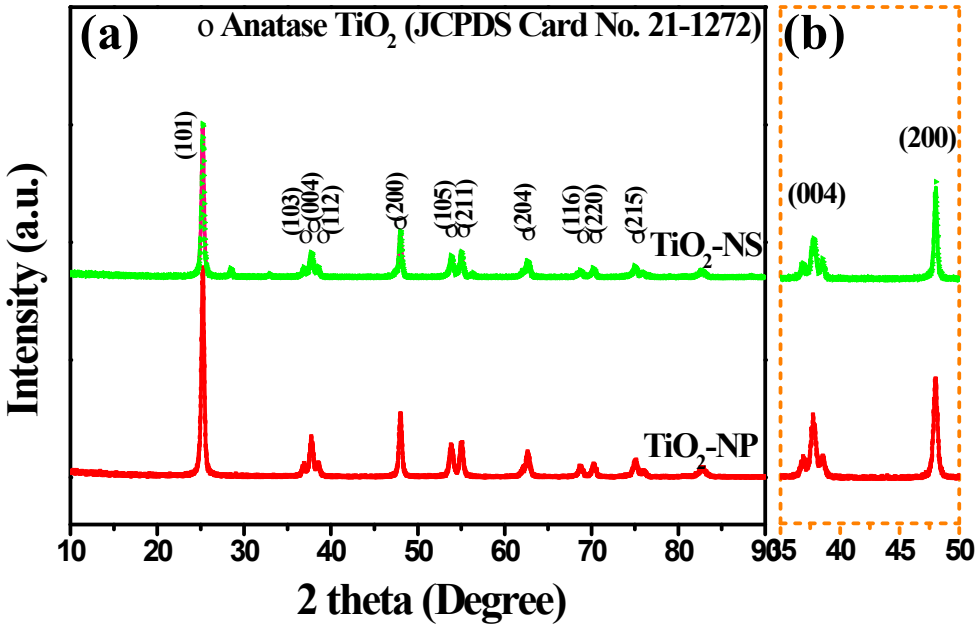

Fig. S1 (a) XRD patterns of TiO_2-NP and TiO_2-NS catalysts. (b) The enlarged part of (a) from 35 to 50 degree.

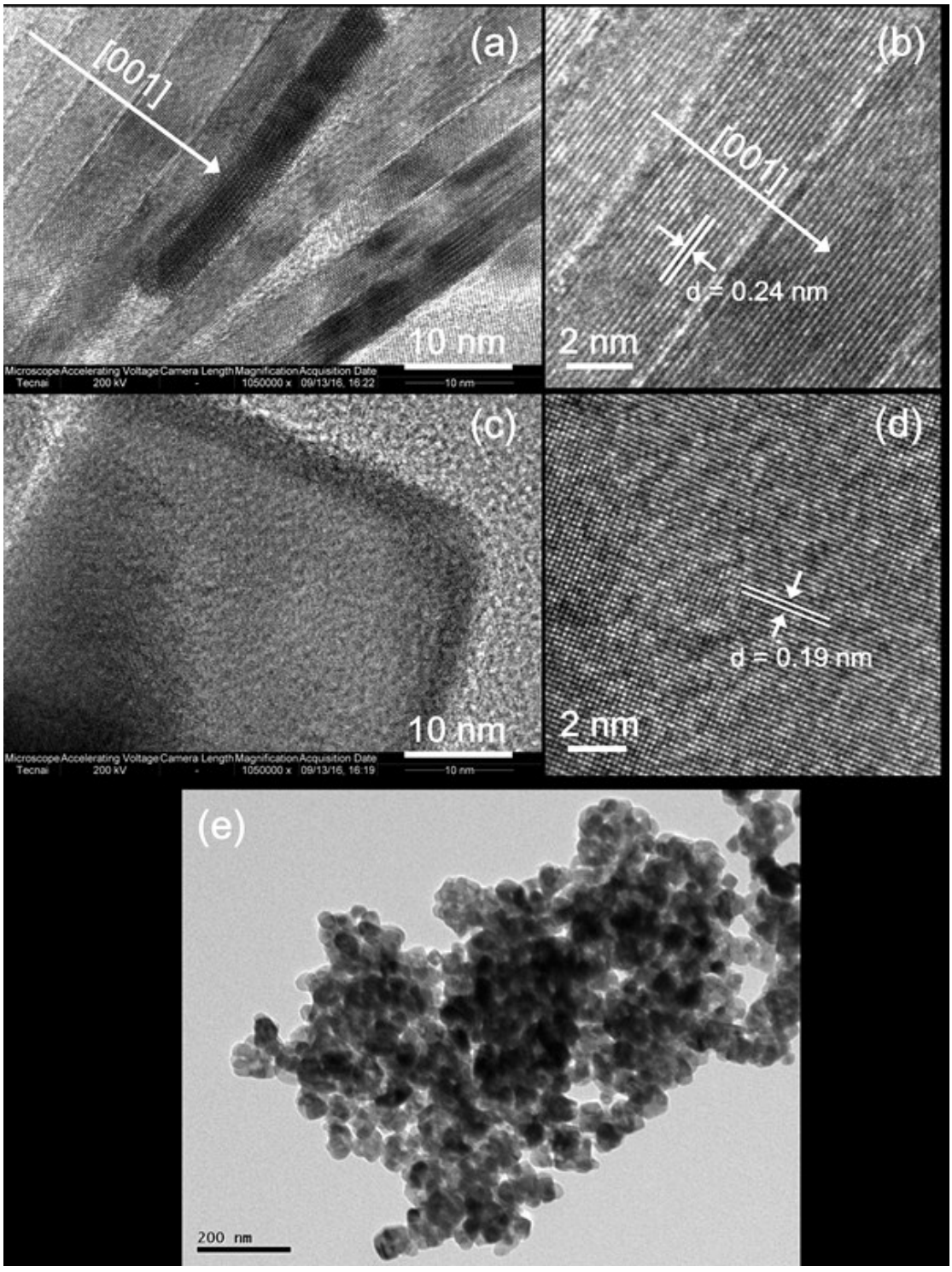

Fig. S2 (a) and (c) are the HRTEM images of TiO_2-NS. (b) and (d) are the enlarged parts of (a) and (c). (e) is the TEM image of TiO_2-NP.

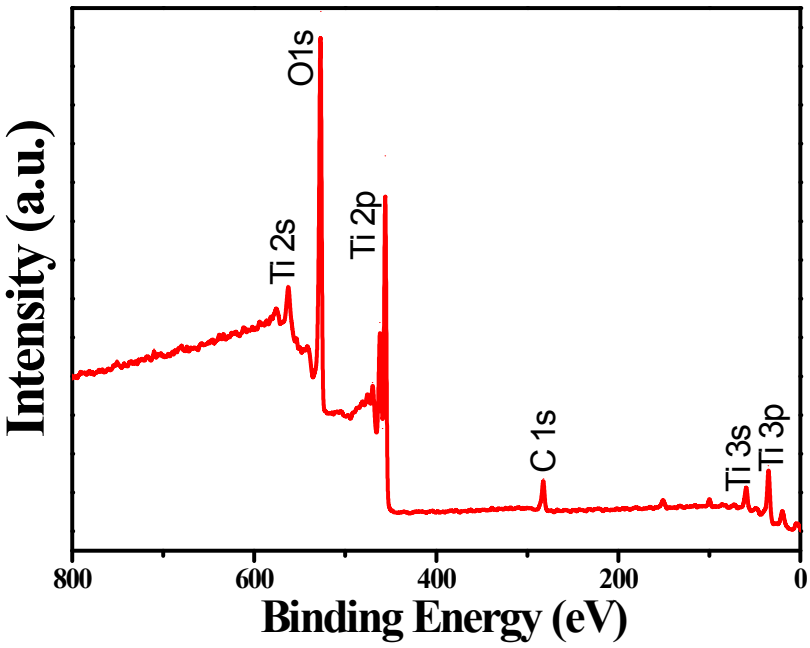

Fig. S3 The full scan XPS spectra of TiO_2-NS catalysts.

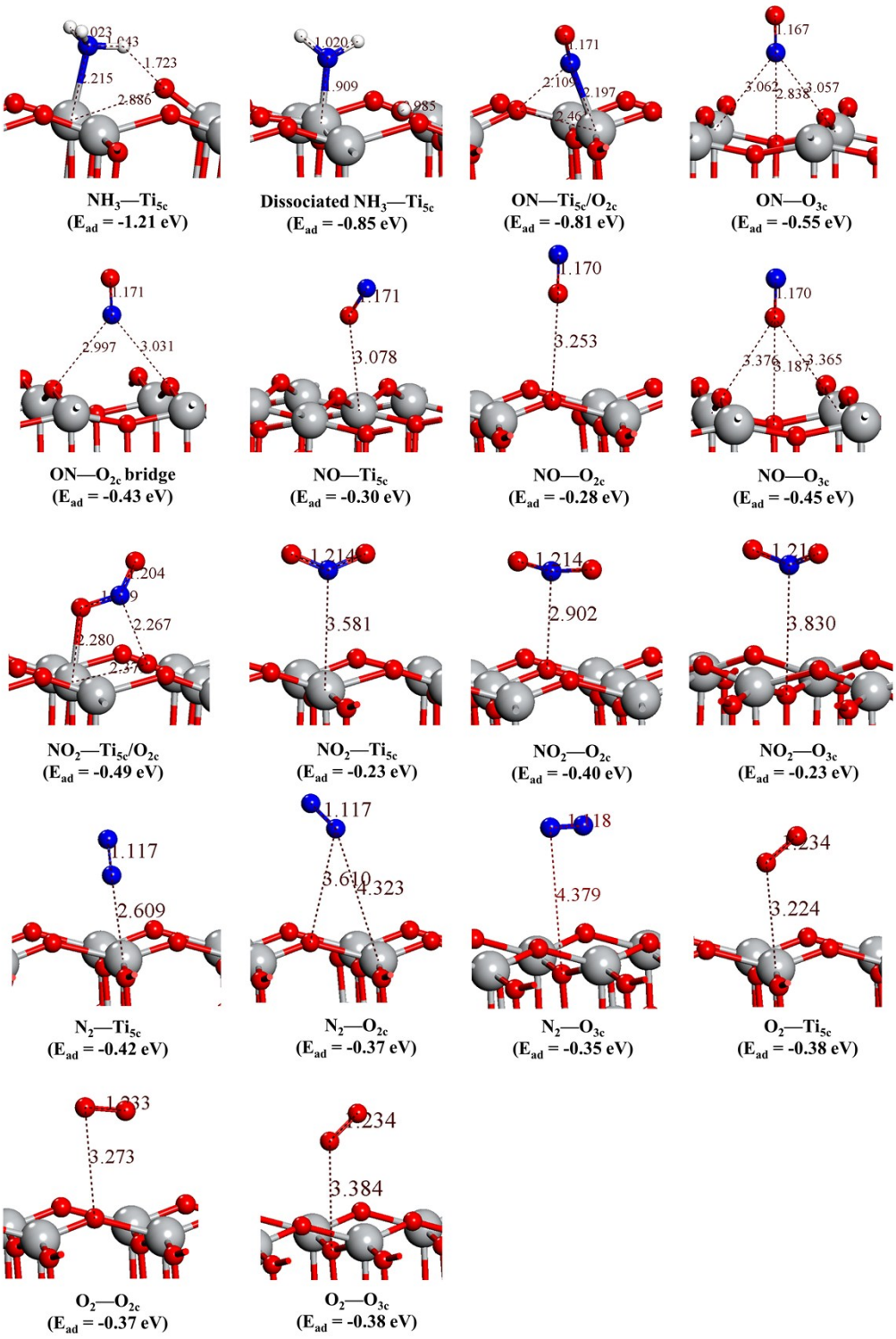

Fig. S4. Possible adsorption configurations with the distances in Å of gas adsorption on the anatase-TiO_2 (001) surface

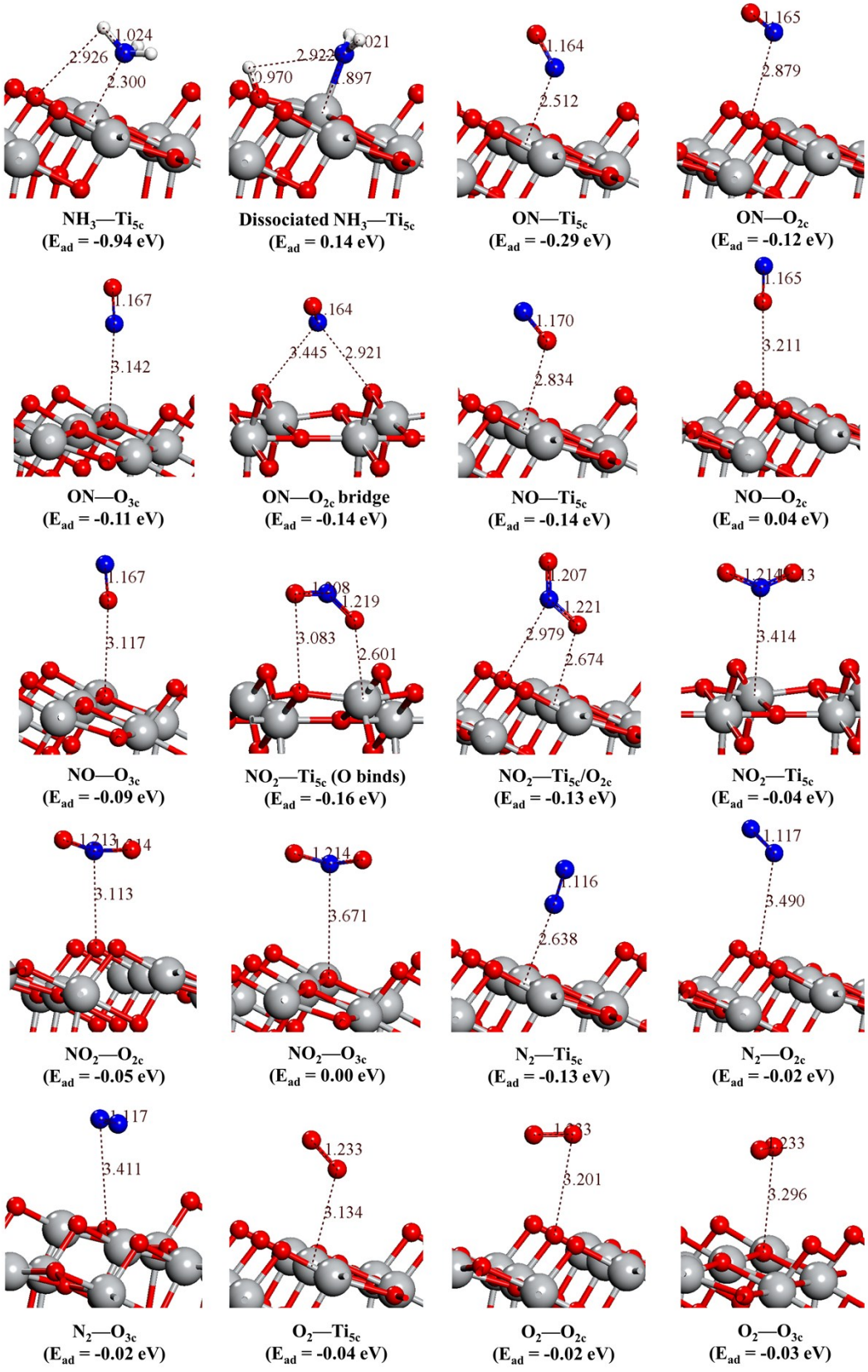

Fig. S5. Possible adsorption configurations of gas adsorption with the distances in Å on the anatase-TiO_2 (101) surface

Table S1: All possible adsorption modes of gases adsorbed on the anatase TiO_2 (001) surface with their calculated adsorption energy (E_{ad}) in eV/molecule

Adsorbate/TiO_2 (001)	E_{ad} (eV/moledule)	
	This work	**Ref.**
NH_3/TiO_2 (001)		
Ti_{5c} site	-1.20	-1.16[a], -1.09[b]
O_{2c} or O_{3c} sites	NH_3 moves to Ti_{5c} site	
Dissociated NH_3*	-0.85	
NO/TiO_2 (001)		
N of NO binding		
ON—Ti_{5c} and O2c sites	-0.81	-0.80[c]
ON—O_{3c} site	-0.55	
ON—O_{2c} bridge	-0.43	
O of NO binding		
NO—Ti_{5c} site	-0.30	-0.12 [c]
NO—O_{2c} site	-0.28	
N-O—O_{3c} site	-0.45	
NO_2/TiO_2 (001)		
Ti_{5c}/O_{2c} site	-0.49	
Ti_{5c} site	-0.23	
O_{2c} site	-0.40	
O_{3c} site	-0.23	
N_2/TiO_2 (001)		
Ti_{5c} site	-0.42	
O_{2c} site	-0.37	
O_{3c} site	-0.35	
O_2/TiO_2 (001)		
Ti_{5c} site	-0.38	
O_{2c} site	-0.37	
O_{3c} site	-0.38	

* One H form hydroxyl group the nearest O_{2C} atom of the TiO_2 (001) surface,

[a]The [1x1] slabs with two Ti layers of the (001) model and the (101) model[1]

[b]The [2x2] slabs with four Ti layers of the (001) model[2]

[c]The [2x2] slabs with four Ti layers of the (001) model[3]

[d]The [1x1] of the (001) model with 1/2, 1/3 and 1/6 ML water coverage[4]

Table S2: All possible adsorption modes of gases adsorbed on the anatase TiO_2 (101) surface with their calculated adsorption energy (E_{ad}) in eV/molecule

Adsorbate/TiO_2 (101)	**E_{ad} (eV/amolecule)**	
	This work	**Ref.**
NH_3/TiO_2 (101)		
Ti_{5c} site	-0.94	-0.7[a]
O_{2c} site and O_{3c} site	NH_3 moves to Ti_{5c} site	
Dissociated NH_3	0.14	
NO/TiO_2 (101)		
N termination binding		
ON—Ti_{5c} site	-0.29	-0.25[b]
ON—O_{2c} site	-0.12	+0.54 [b]
ON—O_{3c} site	-0.11	
O termination binding		
NO—Ti_{5c} site	-0.14	-0.19 [b]
NO—O_{2c} site	0.04	
NO—O_{3c} site	-0.09	
NO_2/ TiO_2 (101)		
Ti_{5c} site (O binds)	-0.16	
Ti_{5c}/O_{2c} site	-0.13	
Ti_{5c} site	-0.04	
O_{2c} site	-0.05	
O_{3c} site	0.00	
N_2/ TiO_2 (101)		
Ti_{5c} site	-0.13	
O_{2c} site	-0.02	
O_{3c} site	-0.02	
O_2/ TiO_2(101)		
Ti_{5c} site	-0.04	
O_{2c} site	-0.02	
O_{3c} site	-0.03	

[a]The [1x1] slabs with two Ti layers of (001) model and the (101) model[1]

[b]The [2x2] slabs with two Ti layers of the (101) model[3]

References

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