Theoretical insight into H_2O impact on V_2O_5/TiO_2 catalysts for selective catalytic reduction of NO_x Supporting Information

Table S1 Values of *H* and *S* used for calculating the chemical potential.

Molecule	Temperature (K)	*H* (kJ·mol^{-1})	*S* (J·K^{-1}·mol^{-1})
H_2O	0	-9.904	0.000
	100	-6.615	152.388
	200	-3.282	1.800
	300	0.062	189.042
	400	3.452	198.788
	500	6.925	206.534
	600	10.501	213.052
	700	14.192	218.739
	800	18.002	223.825
	900	21.938	228.459
	1000	26.000	232.738
NH_3	0	-10.045	0.000
	100	-6.737	155.840
	200	-3.394	178.990
	300	0.066	192.995
	400	3.781	203.663
	500	7.819	212.659
	600	12.188	220.615
	700	16.872	227.829
	800	21.853	234.476

	900	27.113	240.669
	1000	32.637	246.486

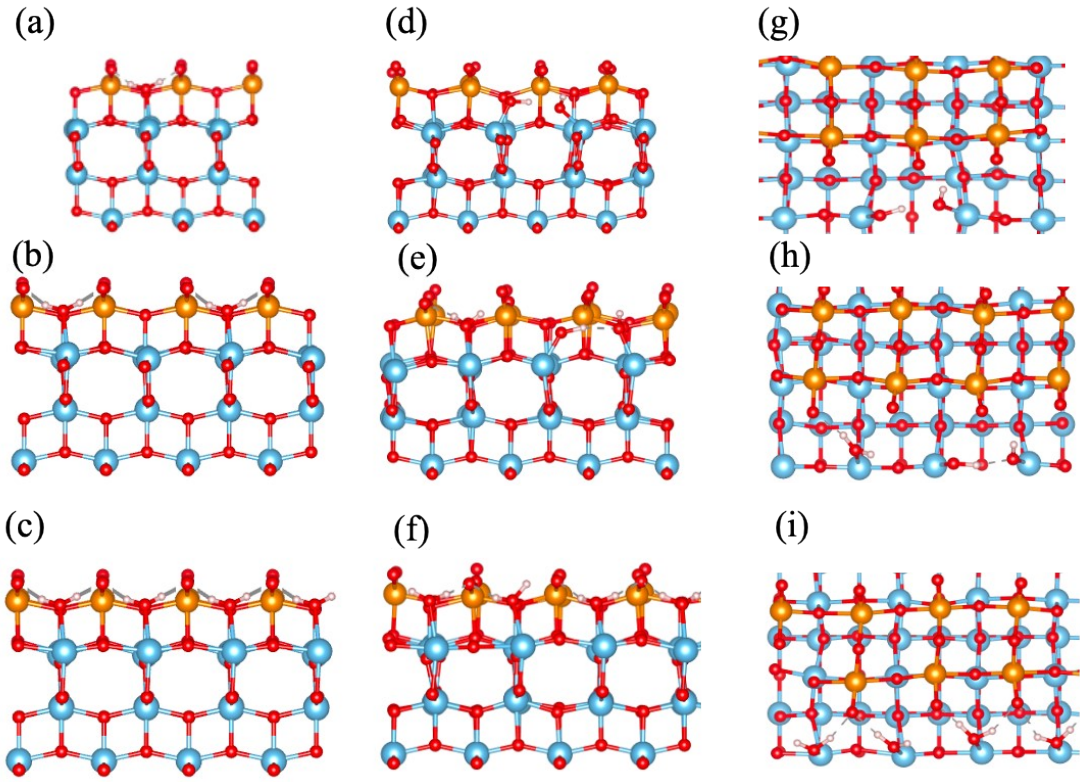

Figure S1 Molecule dynamic simulation of model sub-1-H_2O, sub-2-H_2O,and sub-4-H_2O at 373K for 4000fs; (a)-(c): Side view of sub-1-H_2O, sub-2-H_2O, sub-4-H_2O before molecular dynamic simulation; (d)-(f): Side view of sub-1-H_2O, sub-2-H_2O, sub-4-H_2O after molecular dynamic simulation; (g)-(i): Top view of sub-1-H_2O, sub-2-H_2O, sub-4-H_2O after molecular dynamic simulation; Red are oxygen atoms, blue are titanium atoms, orange are vanadium atoms, light pink are hydrogen atoms.