Supplementary information

Title: Rational Selection of $Fe_2V_4O_{13}$ over $FeVO_4$ as a Preferred Active Site on Sb-Promoted TiO_2 for Catalytic NO_X Reduction with NH_3

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Table S1 Locations and relative abundance of surface Fe, V, and O species for Fe_1/TiO_2 and Fe_2/TiO_2. Values with *italic* indicate location of surface species (eV), whereas values in parentheses indicate relative abundance of surface species (mol. %).

	Fe 2p $_{3/2}$		V 2p $_{3/2}$		O 1s		
	Fe^{3+} [a]	$Fe^{\delta+}$ [a]	V^{5+} [a]	V^{4+} [a]	O'_{α} [a]	O_{α} [a]	O_{β} [a]
Fe_1/TiO_2	*710.9*	*713.3*	*517.3*	*516.2*	*532.6*	*531.2*	*530.0*
	(49.7)	(50.3)	(73.1)	(26.9)	(5.0)	(12.6)	(82.4)
Fe_2/TiO_2	*711.4*	*713.7*	*517.1*	*516.0*	*532.6*	*531.0*	*530.0*
	(42.2)	(57.8)	(68.6)	(31.4)	(0.1)	(20.0)	(79.9)

[a] via deconvolution of XP spectra.

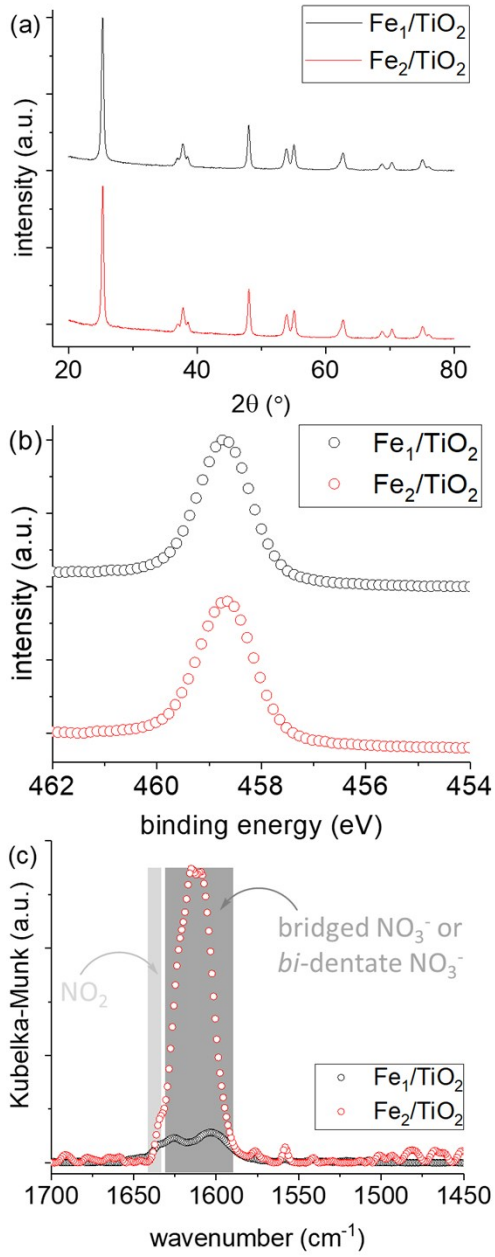

Fig. S1 (a) XRD patterns of Fe_X/TiO_2 catalysts. (b) XP spectra of Fe_X/TiO_2 catalysts in Ti $2p_{3/2}$ regime. (c) Background-subtracted *in situ* DRIFT spectra of Fe_X/TiO_2 catalysts after saturating the surfaces with NO (1000 ppm) and O_2 (3 vol. %) at 220 °C for 30 minutes. Prior to DRIFT runs, the surfaces are initially purged with O_2 and N_2 at 400 °C for an hour. Grey-shaded regimes are assigned to N-O vibrations of multiple NO/O_2-driven species chemisorbed on the surfaces.

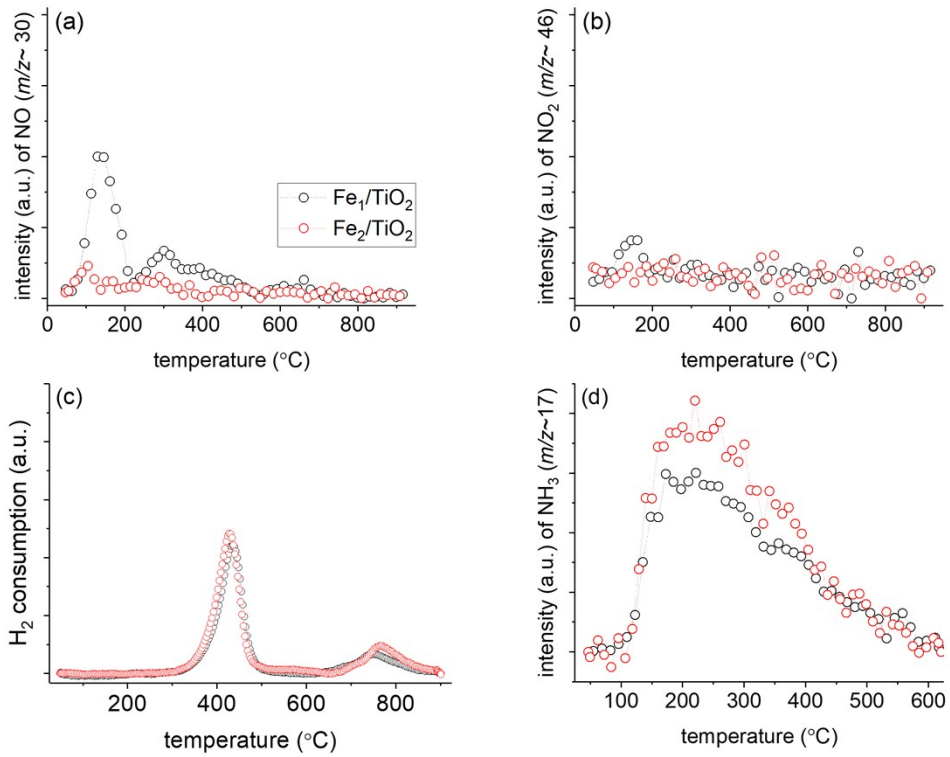

Fig. S2 Profiles of NO-TPD (a for NO desorbed; b for NO_2 evolved), H_2-TPR (c), and NH_3-TPD (d) for Fe_X/TiO_2 catalysts.

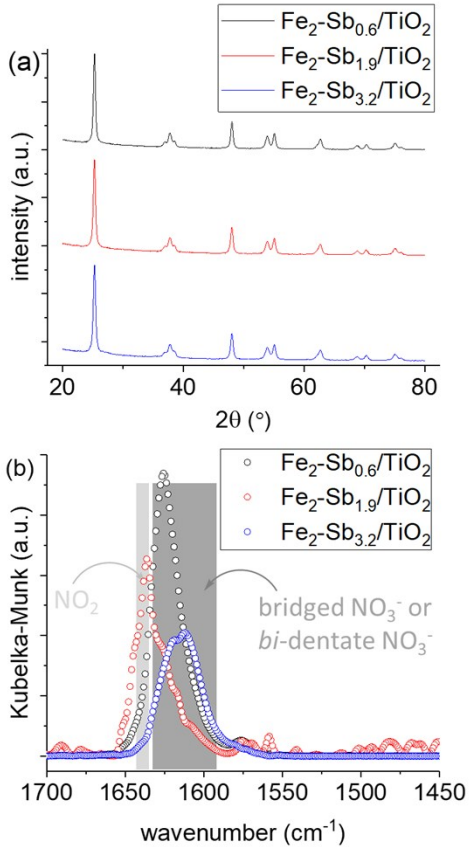

Fig. S3 (a) XRD patterns of Fe_2-Sb_Y/TiO_2 catalysts. (b) Background-subtracted *in situ* DRIFT spectra of Fe_2-Sb_Y/TiO_2 catalysts after saturating the surfaces with NO (1000 ppm) and O_2 (3 vol. %) at 220 °C for 30 minutes. Prior to DRIFT runs, the surfaces are initially purged with O_2 and N_2 at 400 °C for an hour. Grey-shaded regimes are assigned to N-O vibrations of multiple NO/O_2-driven species chemisorbed on the surfaces.

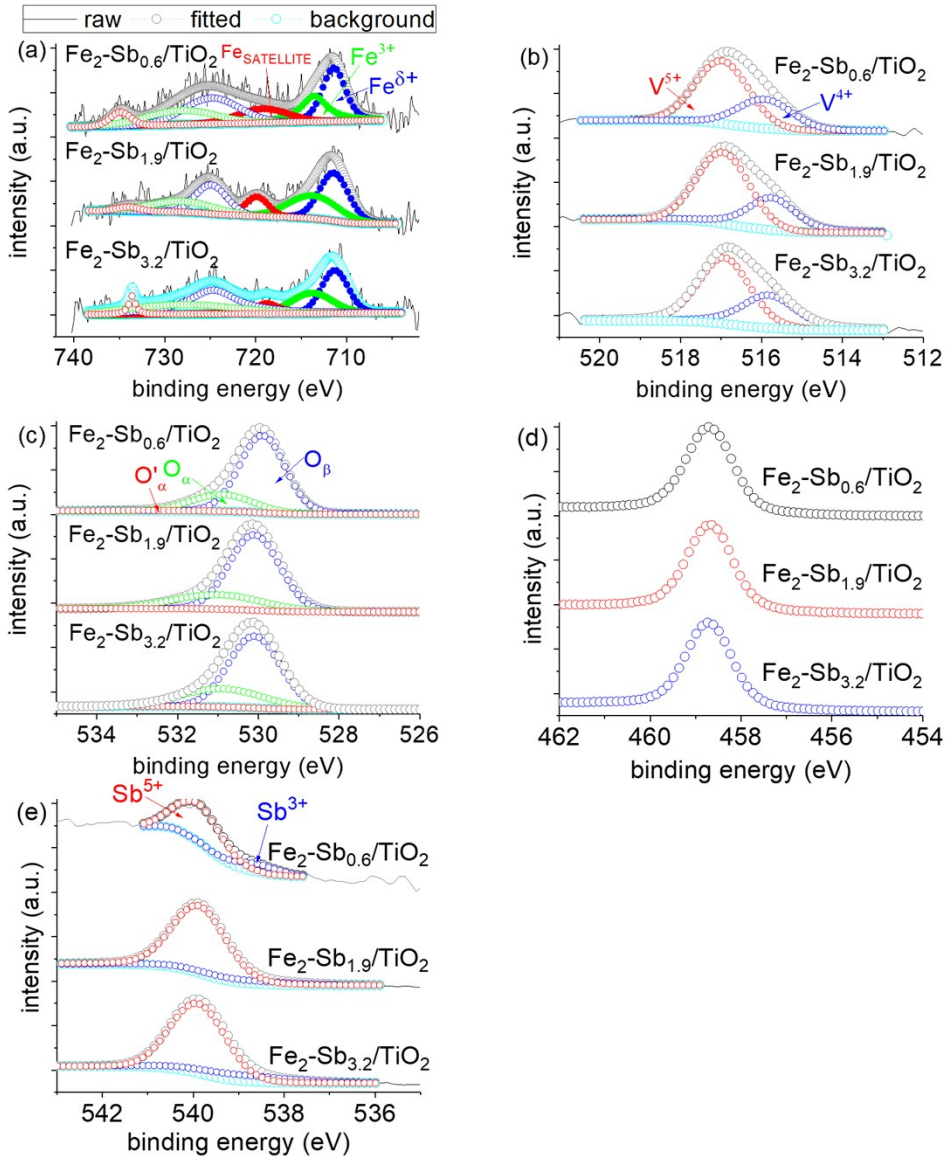

Fig. S4 XP spectra of Fe_2-Sb_Y/TiO_2 catalysts in (a) Fe 2p, (b) V 2p $_{3/2}$, (c) O 1s, (d) Ti 2p $_{3/2}$, and (e) Sb 3d $_{3/2}$ regimes. In (a), solid and empty symbols indicate surface Fe species in Fe 2p $_{3/2}$ and Fe2p $_{1/2}$ regimes, respectively.

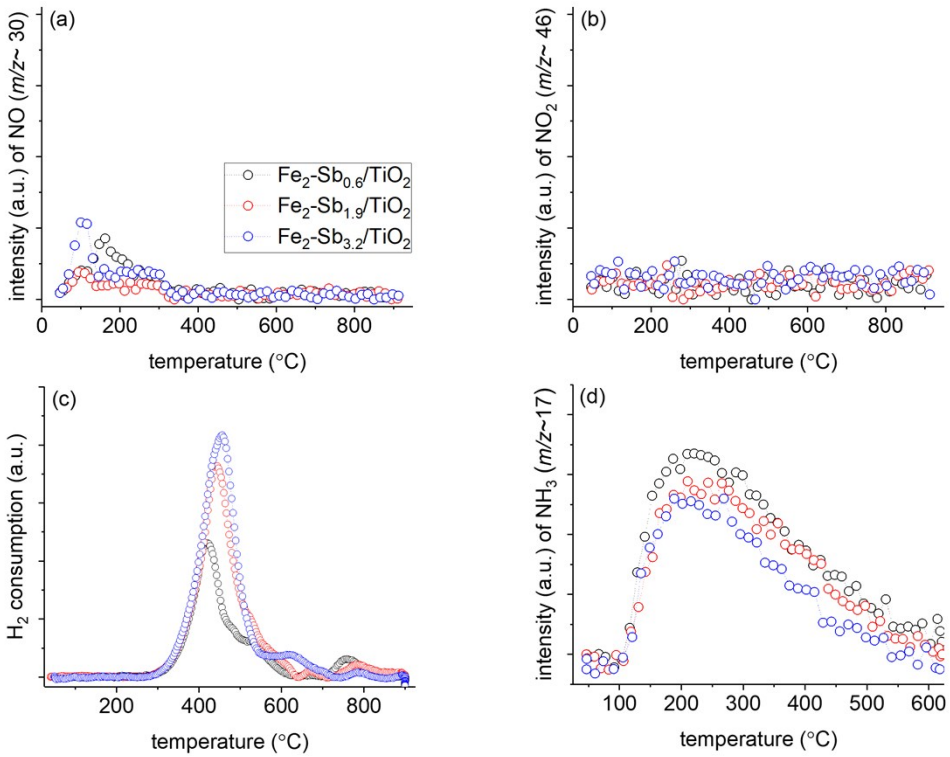

Fig. S5 Profiles of NO-TPD (a for NO desorbed; b for NO_2 evolved), H_2-TPR (c), and NH_3-TPD (d) for Fe_2-Sb_Y/TiO_2 catalysts.

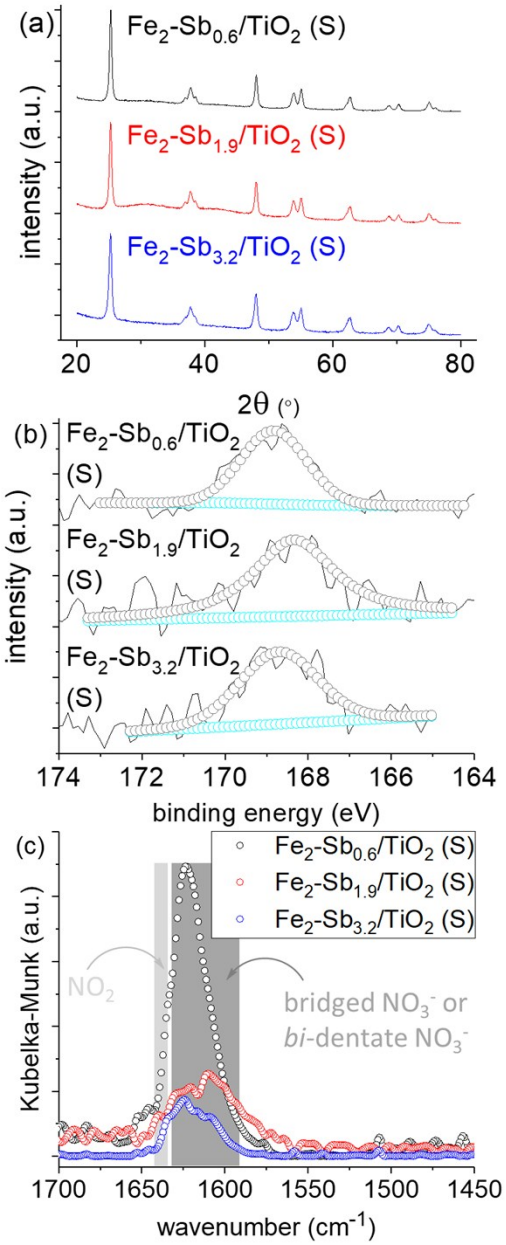

Fig. S6 (a) XRD patterns of Fe_2-Sb_Y/TiO_2 (S) catalysts. (b) XP spectra of Fe_2-Sb_Y/TiO_2 (S) catalysts in S 2p regime. (c) Background-subtracted *in situ* DRIFT spectra of Fe_2-Sb_Y/TiO_2 (S) catalysts after saturating the surfaces with NO (1000 ppm) and O_2 (3 vol. %) at 220 °C for 30 minutes. Prior to DRIFT runs, the surfaces are initially purged with O_2 and N_2 at 400 °C for an hour. Grey-shaded regimes are assigned to N-O vibrations of multiple NO/O_2-driven species chemisorbed on the surfaces.

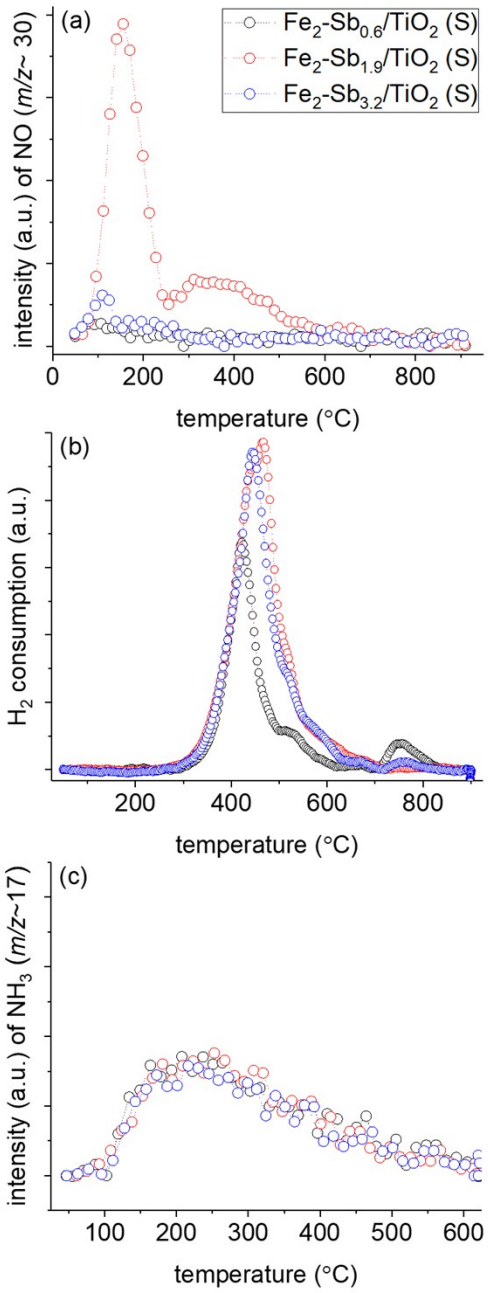

Fig. S7 Profiles of NO-TPD (a for NO desorbed), H_2-TPR (b), and NH_3-TPD (c) for Fe_2-Sb_Y/TiO_2 (S) catalysts.