

Supplementary data

Site-specific catalytic activities to facilitate solvent-free aerobic oxidation of cyclohexylamine to cyclohexanone oxime over highly efficient Nb-modified SBA-15 catalysts

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Table S1 Some XPS features of samples with different Nb contents.

Catalyst	Binding energy [eV]				Nb/Si atomic ratio	
	O 1s	Si 2p	Nb 3d _{3/2}	Nb 3d _{5/2}	Surface ^[a]	Bulk ^[b]
SBA-15	533.02	103.83	-	-	-	-
Nb/SBA-15/1im	533.40	104.21	210.58	208.49	0.011	0.010
Nb/SBA-15/3im	533.55	103.97	210.48	207.94	0.029	0.030
Nb/SBA-15/5im	533.48	103.94	210.78	208.06	0.043	0.046
Nb/SBA-15/3co	533.56	103.56	210.78	207.97	0.016	0.083
Nb ₂ O ₅	530.2	-	209.61	207.02	-	-

[a] Determined by XPS analysis. [b] Determined by X-ray fluorescence.

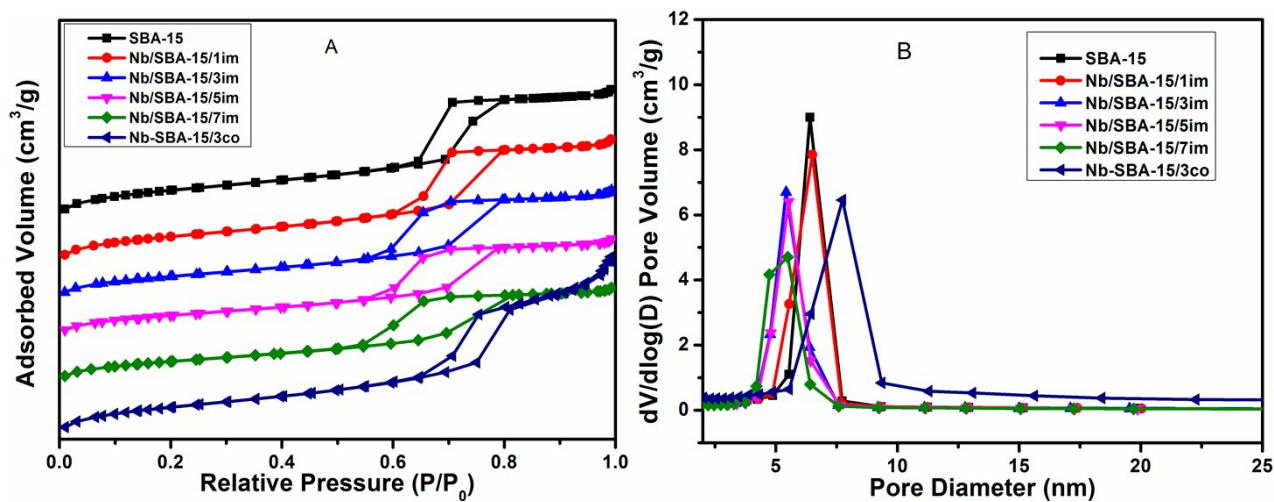


Fig. S1. N_2 adsorption-desorption isotherms (A) and pore diameter distribution (B) of samples.

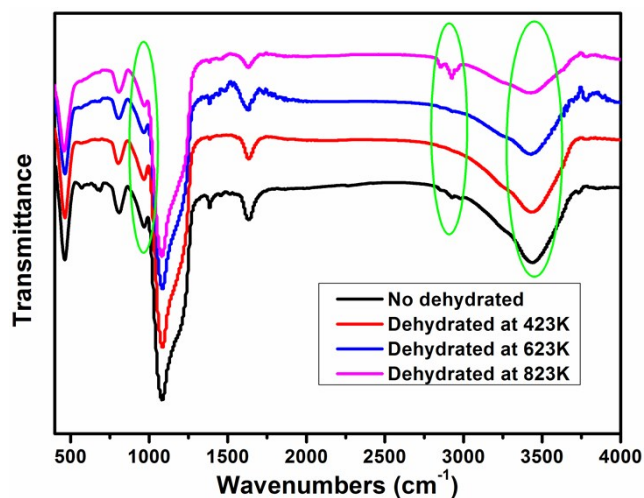


Fig. S2 FT-IR spectra of Nb/SBA-15/3im samples at at different dehydration temperatures.

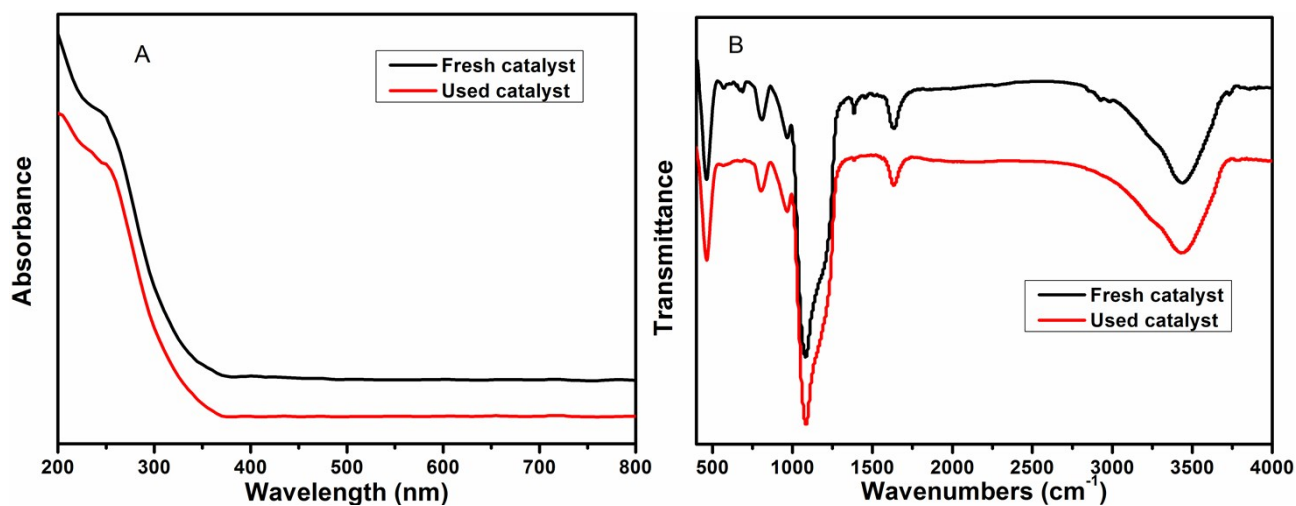


Fig. S3 Diffuse reflectance UV-Vis (A) and FT-IR spectra (B) of the fresh and used Nb/SBA-15/3im catalysts.

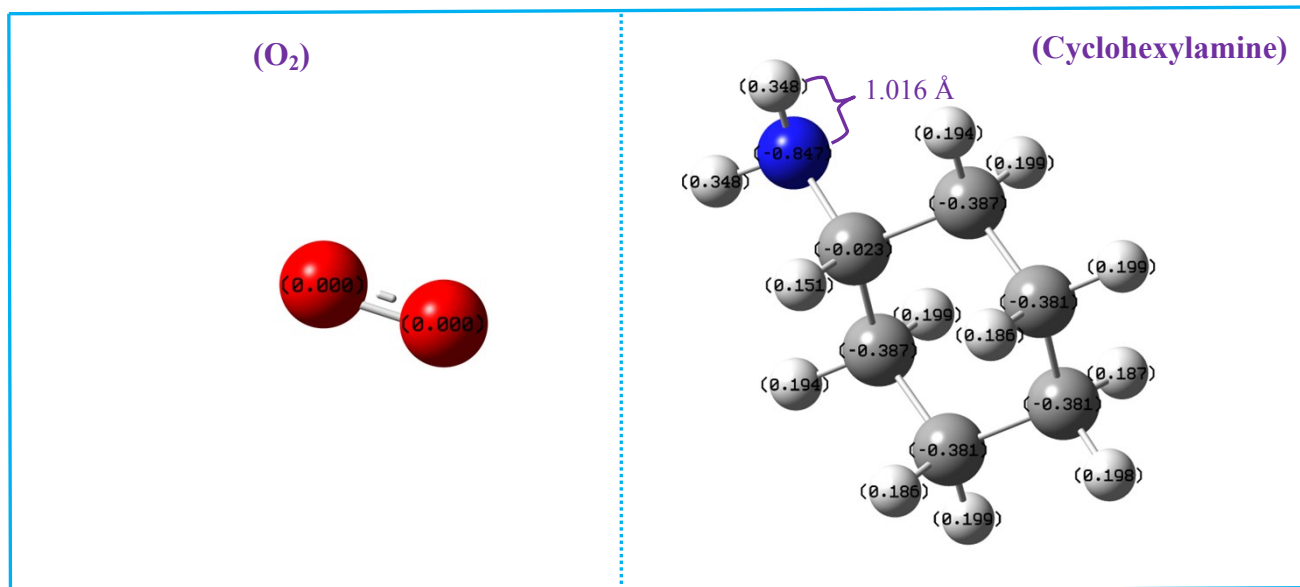


Fig. S5 Computational structures of oxygen (a) and cyclohexylamine (b).

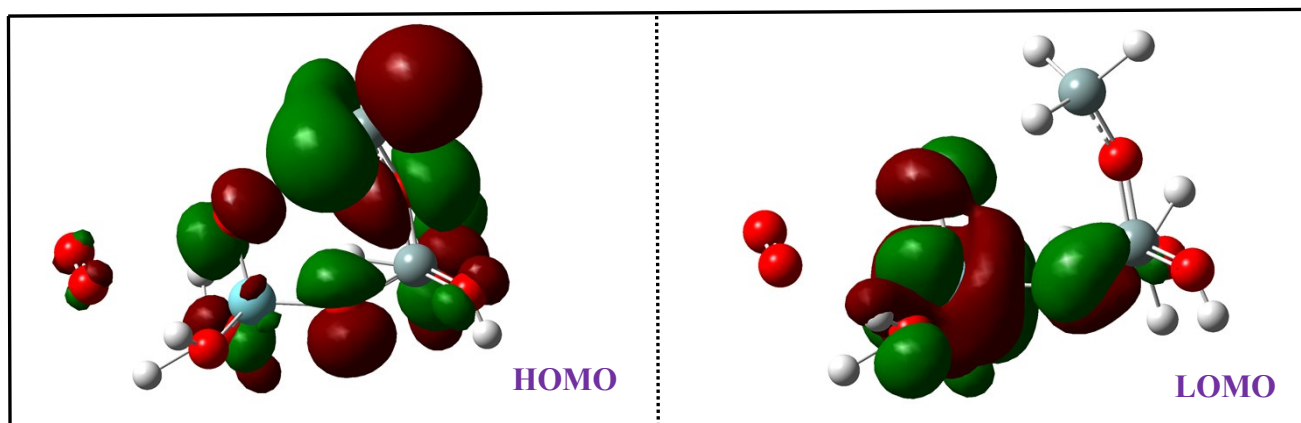


Fig. S6 The HOMO and LOMO orbitals of optimized models for the isolated Nb species grafted onto SBA-15 surface (a-o) with the interactions between O₂ and the redox Nb sites.