Electronic Supplementary Material (ESI) for Catalysis Science & Technology.
This journal is © The Royal Society of Chemistry 2015

Insights into the effects of steam on propane dehydrogenation over Pt/Al_2O_3 catalyst

Yu-Ling Shan[1], Yi-An Zhu[1], Zhi-Jun. Sui[1,*], De Chen[2] and Xing-Gui Zhou[1]

[1]State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai 200237, P. R. China

[2]Department of Chemical Engineering, Norwegian University of Science and Technology, N-7491, Trondheim, Norway

Corresponding author:zhjsui@ecust.edu.cn

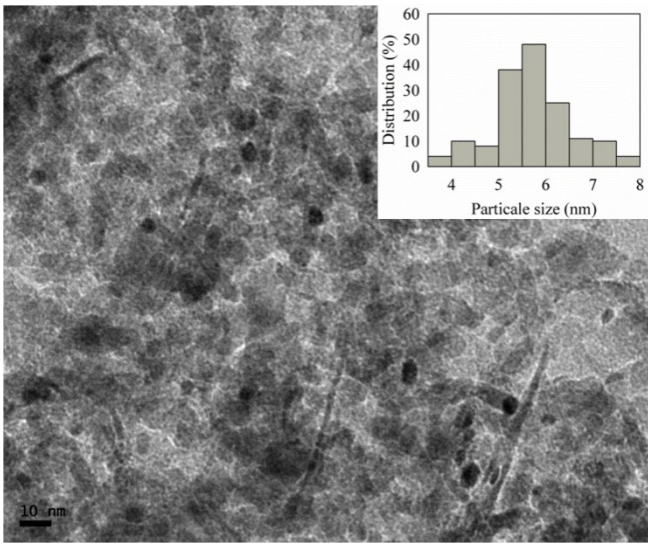

Fig. S1. TEM image of prepared $Pt/\gamma\text{-}Al_2O_3$ catalyst, the in-set shows the particle size distribution of Pt.

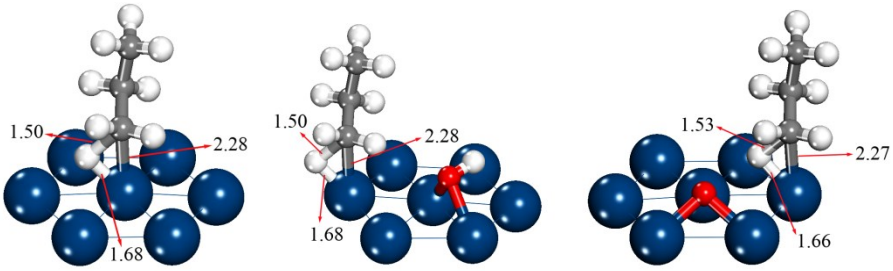

Fig. S2. Transition states structures of propane dehydrogenation at a) clean Pt(111) surface, OH*Pt(111) surface and O*Pt(111) surface.

Table S1 Adsorption energies and geometries of hydroxyl and oxygen atom on Pt(111) surface

species	Adsorption Sites	$\triangle E_{ads}$ (eV)
Hydroxyl (-OH)	Atop	-2.25
	Bridge	-2.34
Oxygen atom (-O)	Atop	-3.13
	Bridge	-4.40
	Fcc	-4.41