

Supporting Information

Controllable deposition of Pt nanoparticles into KL zeolite by atomic layer deposition for highly efficient reforming of *n*-heptane to aromatics

**Dan Xu^{a,c}, Baoshan Wu^{a,b,*}, Pengju Ren^{a,b}, Shuyuan Wang^{a,c}, Chunfang Huo^{a,b},
Bin Zhang^a, Wenping Guo^b, Lihua Huang^b, , Xiaodong Wen^{a,b}, Yong Qin^a, Yong
Yang^{a,b,*}, Yongwang Li^{a,b,*}**

^a State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of
Sciences, Taiyuan 030001, People's Republic of China

^b National Energy Research Center for Clean Fuels, Synfuels China Co., Ltd, Beijing 101400,
People's Republic of China

^c University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

*Corresponding authors. +86 010 69667779.
E-mail addresses: wbs@sxicc.ac.cn, yyong@sxicc.ac.cn and ywl@sxicc.ac.cn.

1. Preparation of 0.50 wt% Pt/KL catalyst by incipient wetness impregnation (IWI)

Supported Pt/KL catalyst with 0.50 wt% Pt loading was also prepared by the IWI method. In a typical synthesis, $\text{Pt}(\text{NH}_3)_4\text{Cl}_2$ was weighed, dissolved in de-ionized water, and impregnated over the dry support by slowly dropping the solution under air atmosphere for 12 h. Next, the mixture was dried in an oven at 120 °C overnight and then calcined at 350 °C for 4 h in static air to yield the final catalyst. The catalyst is denoted as 0.50 wt% Pt/KL.

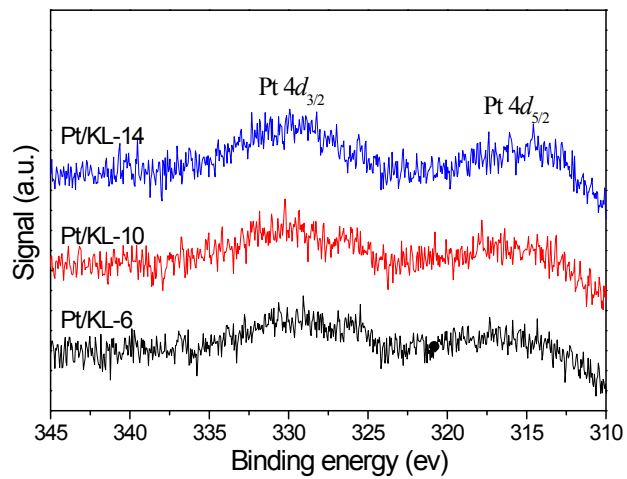


Fig. S1 XPS patterns of Pt4d photoemission spectra of Pt/KL catalysts

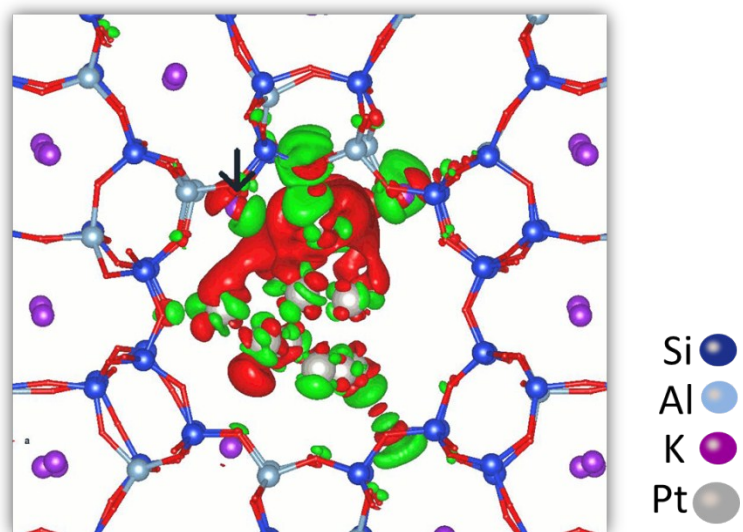


Fig. S2 Charge density difference in a Pt/KL sample

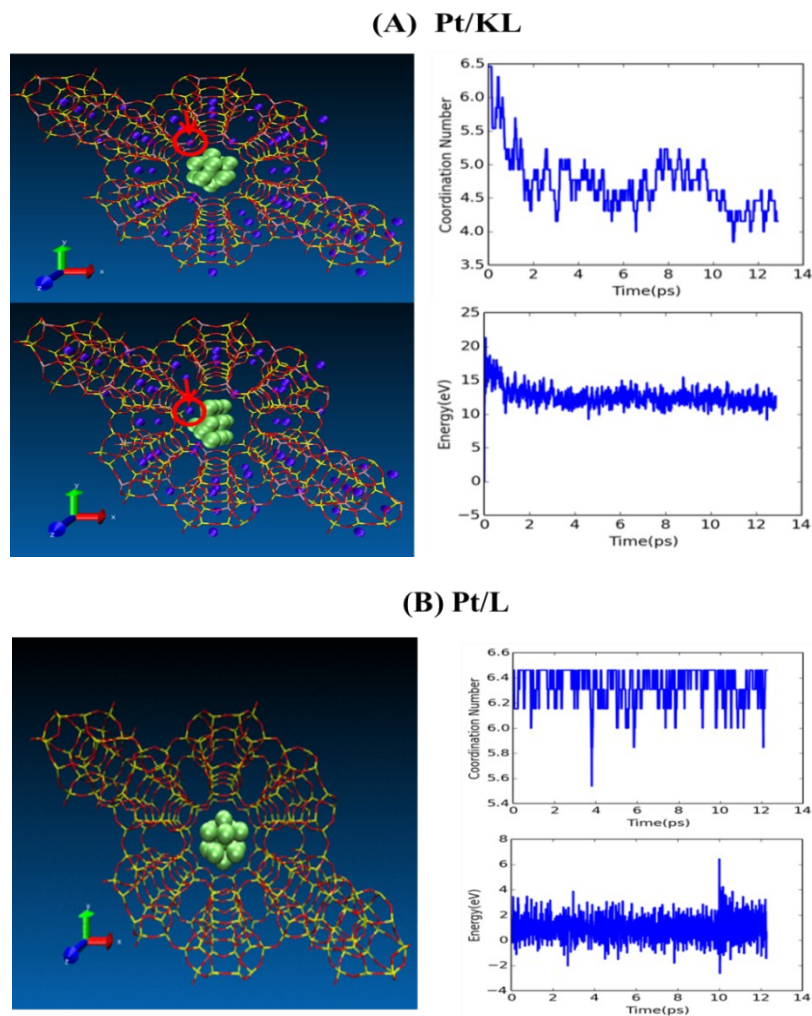


Fig. S3 AIMD simulation of Pt/KL (A) and Pt/L (B) catalysts

Fig. S3 shows the ab initio molecular dynamics (AIMD) simulation about the effect of K^+ cation on the morphology of Pt particle. Fig. S3(A) indicates that Pt particle inside KL zeolite channel could move easily and approach to K^+ cations, which may induce the translocation of K^+ position in the KL zeolite. When K^+ cation is removed from the KL zeolite, Pt particle keeps the isolated structure inside the L zeolite channel (Fig. S3(B)), which has a slight interaction with the zeolite.