Supporting information for

Mechanism of Alkane H/D exchange over Zeolite H-ZSM-5 at Low Temperature: A Combined Computational and Experimental Study

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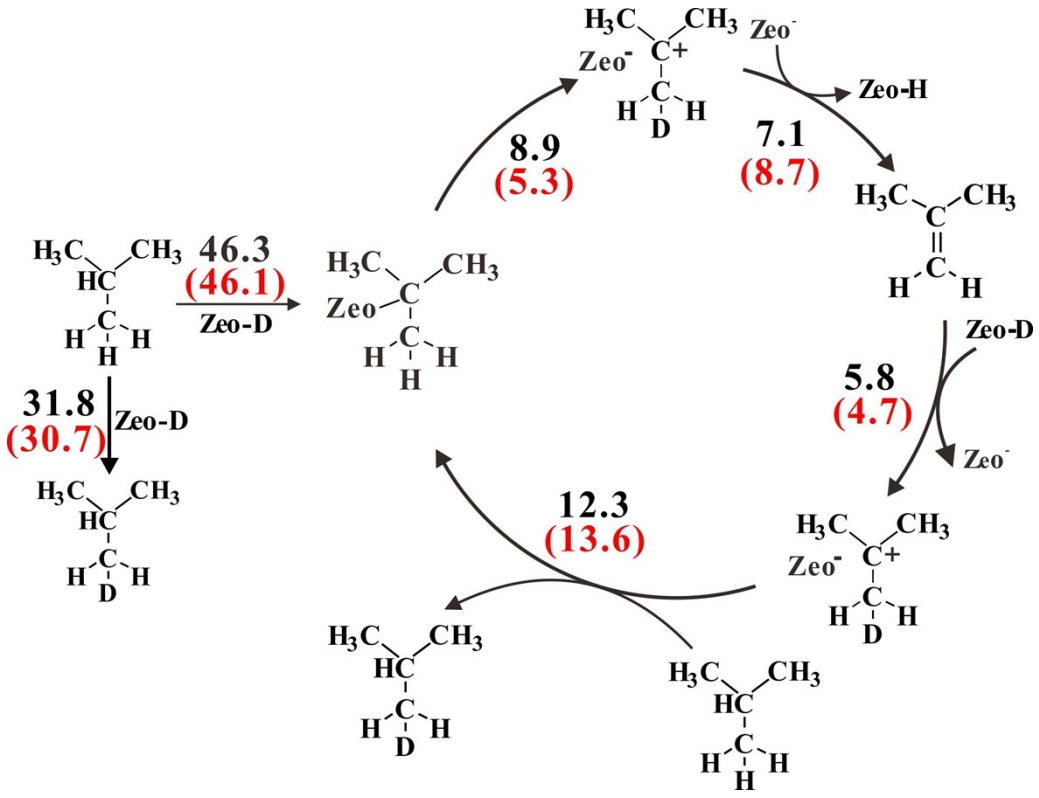
Table S1. The adsorption energy and intrinsic activation barriers (kcal/mol) of isobutane direct H/D exchange over 72T H-ZSM-5 zeolite model with different number of active site atoms treated as high level (See Figure S1) .[a]

	E_{ads}	E_{act}
2T (O_3Si-OH-AlO_3)	-10.9	32.5
8T ($(SiO)_3Si$-OH-$Al(OSi)_3$)	-11.1	31.8
12T ($(SiO)_2(SiO)_3Si$-OH-$Al(OSi)_3(SiO)_2$)	-11.2	31.8

[a] The structure optimizations are performed on the level of ONIOM(m062x/6-31g(d,p):mndo) with the high level atoms relaxing. Based on the optimized structures, the adsorption energy and intrinsic activation barrier are calculated on the level of m062x/6-31g(d,p).



Scheme S1. The activation energy of isobutane H/D exchange in HZSM-5 zeolite at M062X/6-31g(d,p) (in black) and ωB97dx/6-31g(d,p) (in bracket) theoretical levels.

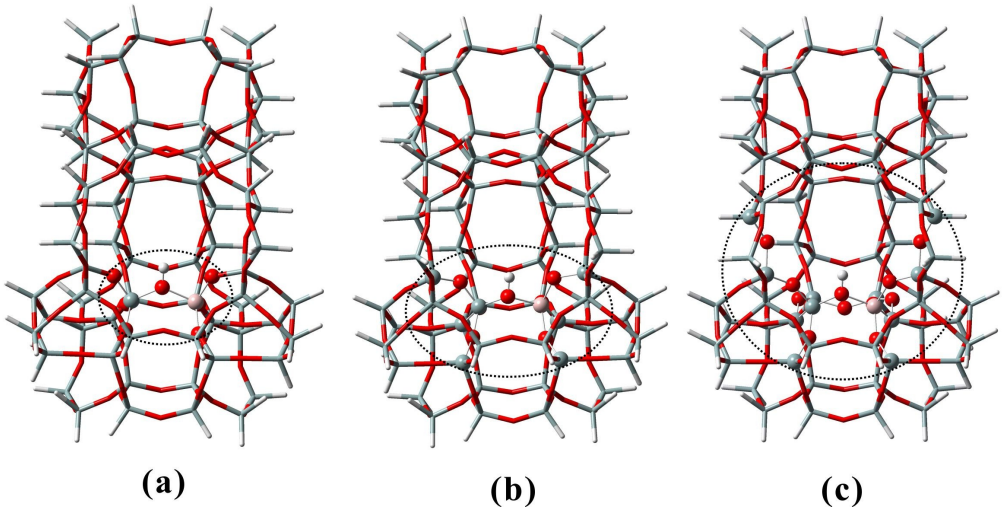


Figure S1 Representation of H-ZSM-5 zeolite by 72T model. The 2T (a), 8T (b) and 12T (c) cluster in the extended cluster models represented as ball and stick view was treated as high-layer atoms during the ONIOM calculations.

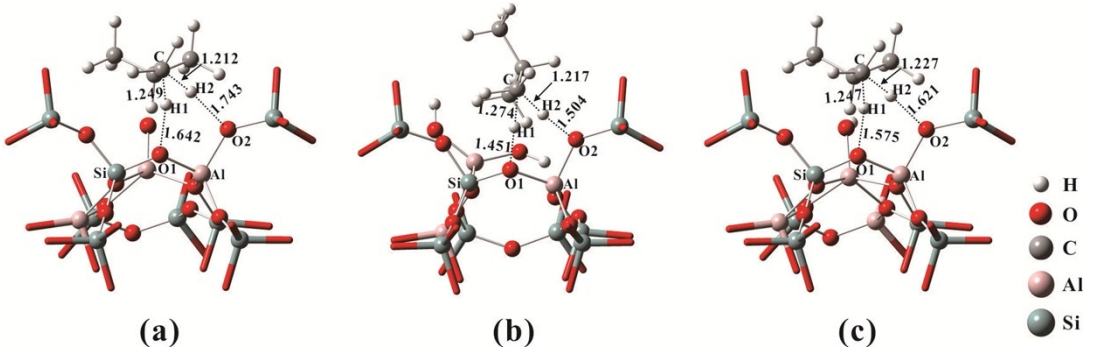


Figure S2. Optimized geometries of transition states (TS) for isobutane direct H/D exchange over EFAL-H-ZSM-5 zeolite with the accessible EFAL species (a) AO^{+}, (b) $Al(OH)_2^{+}$ and (c) $AlOH^{2+}$. Selected interatomic distances (in Å) are indicated.