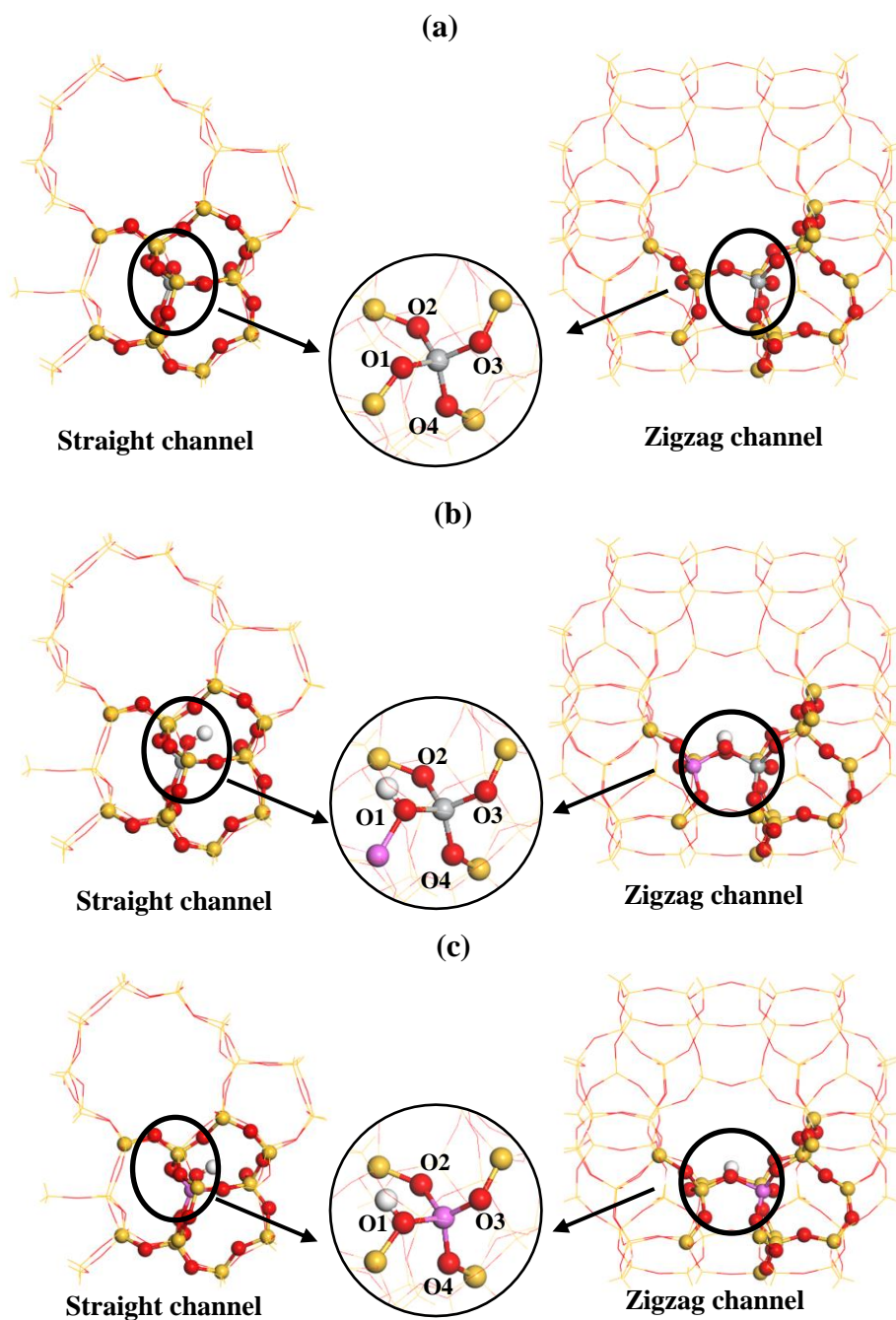


## Supporting Information



**Figure S1.** Optimized structure of the Ti sites models calculated at the QM/MM method. (a) TS-1, (b) Al-TS-1 and (c) ZSM-5. View along the straight channel and zigzag channel. (Ti = lightgray, Si = green, O = red, Al=pink, and H = white).

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