## **Supplementary Material**

## Temperature-Programmed Desorption studies of NH<sub>3</sub> and H<sub>2</sub>O on RuO<sub>2</sub>(110) surface:

## **Effects of Adsorbate Diffusion**

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Figure S1. The illustration of side and top views of adsorption  $NH_3$  on first and second layer of  $RuO_2(110)$  surface.



**Figure S2.** The simulated TPD spectra for (a)  $NH_3$  and (b)  $H_2O$  on  $RuO_2$  (110) surface by our previous study<sup>1</sup>. (Insets are the corresponding experimental TPD spectra taken from Refs.<sup>2, 3</sup>)



**Figure S3.** The obtained  $\theta'(E,T)$  and f(E,T) versus activation energy of 50% ML ammonia on RuO<sub>2</sub>(110) surface at temperature, 500K



**Figure S4.** The guessed and calculated energy distribution with respect to different standard deviation values ( $\sigma = 0.05, 0.10, 0.15$  and 0.20). Red line is the energy distribution we assumed and blue line is the calculated energy distribution from eqn. (9).



Figure S5. The standard deviation vs. RMS plot for determining the optimum energy distribution

## References

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