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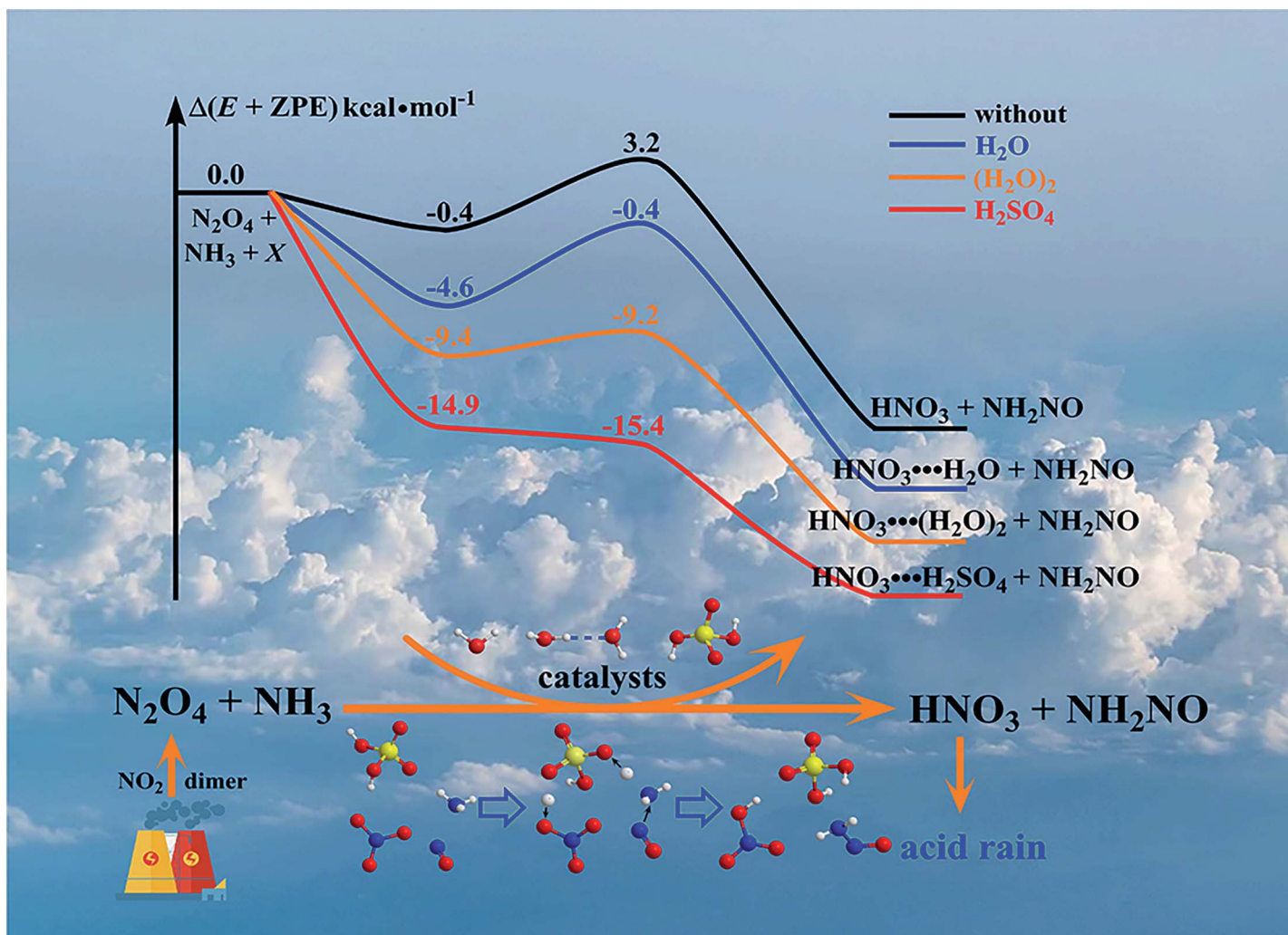
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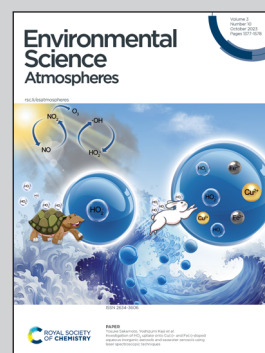


Showcasing research from Professor Tianlei Zhang's laboratory, School of Chemistry & Environment Science, Shaanxi University of Technology, Hanzhong, China.

A possible atmospheric source of  $\text{HNO}_3$ : the ammonolysis reaction of  $t\text{-N}_2\text{O}_4$  in the presence of water monomer, water dimer, and sulfuric acid

The effect of  $\text{H}_2\text{O}$ ,  $(\text{H}_2\text{O})_2$  and  $\text{H}_2\text{SO}_4$  on the ammonolysis of  $t\text{-N}_2\text{O}_4$  to form  $\text{HNO}_3$  was studied by a quantum chemical method and Master equation rate calculations. Results reveal that the ammonolysis of  $t\text{-N}_2\text{O}_4$  with  $(\text{H}_2\text{O})_2$  and  $\text{H}_2\text{SO}_4$  are barrierless or nearly barrierless reactions. Considering the effective rate constant,  $(\text{H}_2\text{O})_2$  outperforms the other catalysts in the range of 280-320 K (0 km). Moreover, the effect of  $\text{H}_2\text{SO}_4$  is obvious at higher altitudes of 5-30 km. In general, this work will give new insights into how the neutral and acidic catalysts affect the formation of  $\text{HNO}_3$ .

As featured in:



See Tianlei Zhang *et al.*, *Environ. Sci.: Atmos.*, 2023, 3, 1407.