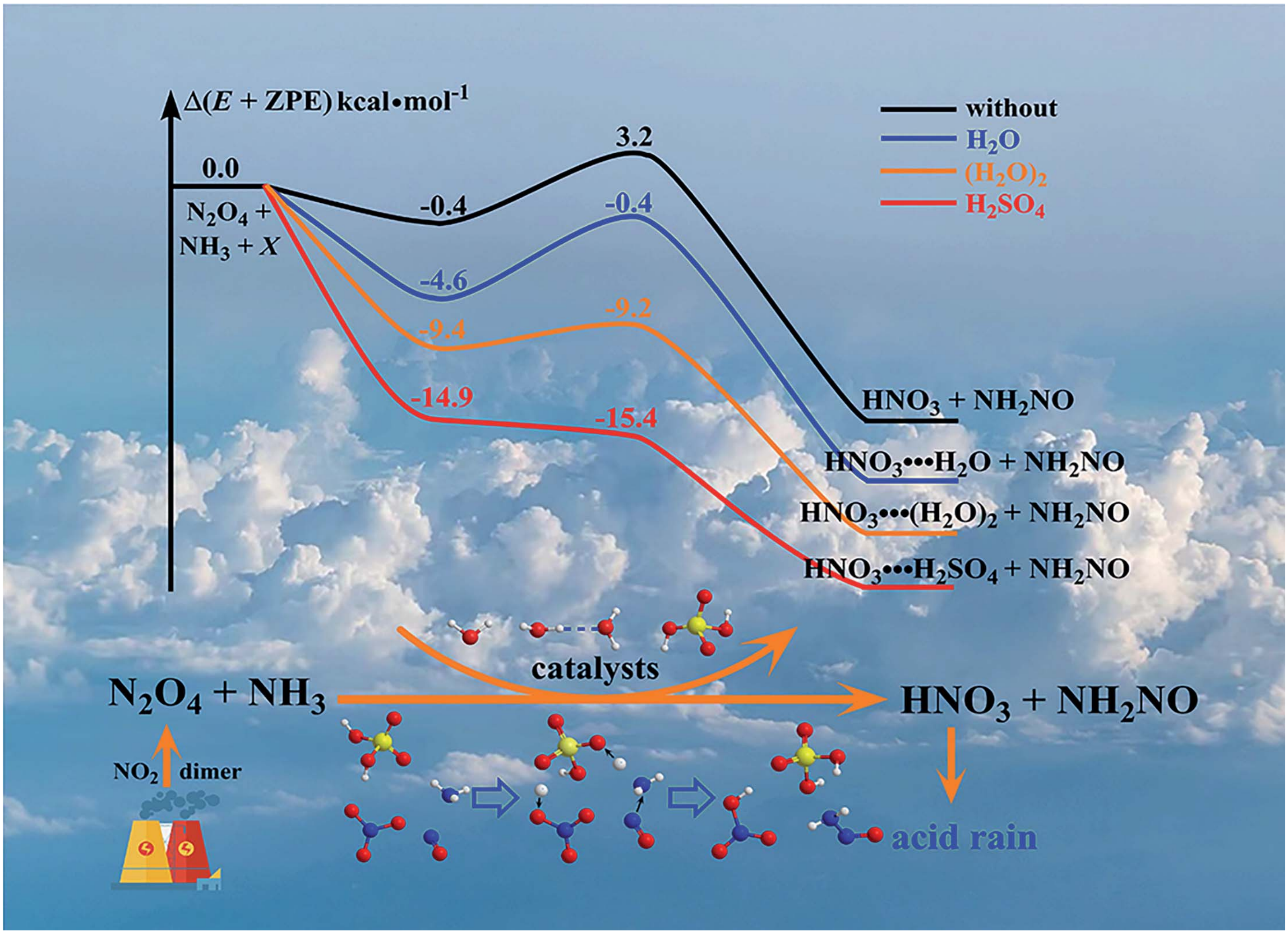

Showcasing research from Professor Tianlei Zhang's laboratory, School of Chemistry & Environment Science, Shaanxi University of Technology, Hanzhong, China.

A possible atmospheric source of HNO_3: the ammonolysis reaction of *t*-N_2O_4 in the presence of water monomer, water dimer, and sulfuric acid

The effect of H_2O, $(H_2O)_2$ and H_2SO_4 on the ammonolysis of *t*-N_2O_4 to form HNO_3 was studied by a quantum chemical method and Master equation rate calculations. Results reveal that the ammonolysis of *t*-N_2O_4 with $(H_2O)_2$ and H_2SO_4 are barrierless or nearly barrierless reactions. Considering the effective rate constant, $(H_2O)_2$ outperforms the other catalysts in the range of 280-320 K (0 km). Moreover, the effect of H_2SO_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 HNO_3.

As featured in:

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

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