

Supporting Information

Catalytic activity of single-atom copper modified reconstructed cerium dioxide (100) surface for Ammonia oxidation: A DFT+U study

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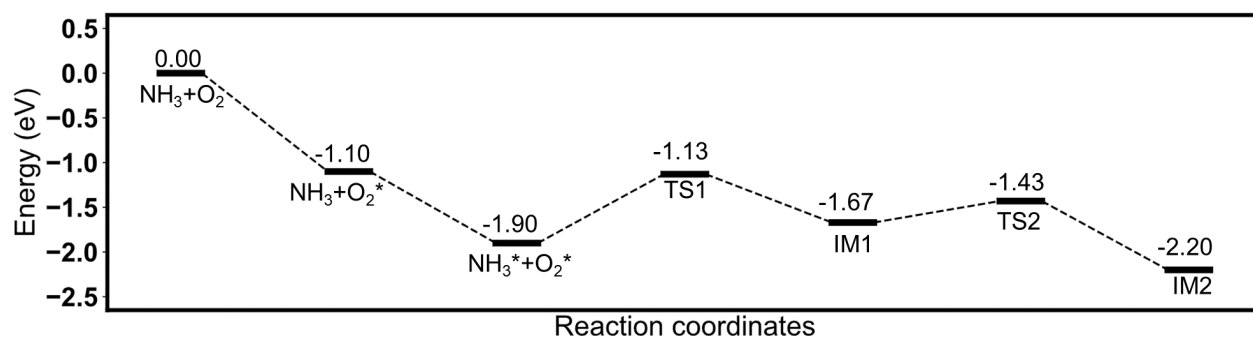


Figure S1. Calculated energy profile of the ammonia dissociation. The state with gas-phase ammonia and oxygen molecules is set to energy zero.

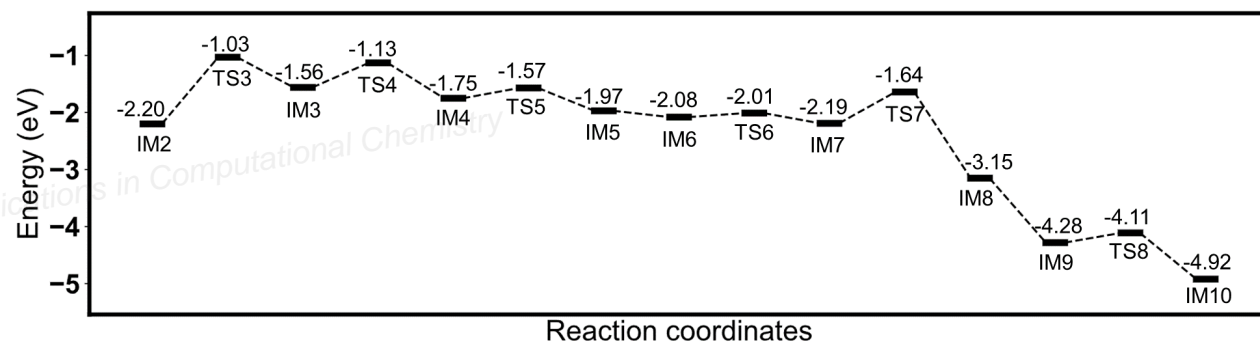


Figure S2. Calculated energy profile of the ammonia oxidation process. The state with the unabsorbed ammonia and oxygen molecules is set to energy zero.