

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: The Supplementary Data file includes the optimized configurations from the density functional theory (DFT) calculations. Particularly, it includes

- The pristine surface of Cu₁-Ti pairs and Ti-Ti pairs.
- The reaction intermediates of path $*NO \rightarrow *NHO \rightarrow *NHOH \rightarrow *NHHOH \rightarrow *NHH$ on Cu₁-Ti pairs and Ti-Ti pairs.