

H₂ dissociation over Ag/Al₂O₃: The first step in hydrogen assisted selective catalytic reduction of NO_x

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Electronic Supplementary Information

Herein we present the calculated low energy structures in the case of molecular and dissociated H₂ adsorption. These are referred to as the initial (I) and final (F) states, respectively. Moreover, the calculated transition state (TS) structures are reported. For the Ag@Al₂O₃(110)-b structure, only the final state is reported as no barrier for dissociation is found in this case. Finally, for clarity, we present the bare Ag@Al₂O₃(110)-a structures. All structures are presented in a top view, besides the Ag@Al₂O₃(110)-a structure which also is given in a side view. Color codes: blue, purple, red, white balls correspond to Ag, Al, O, and H respectively.

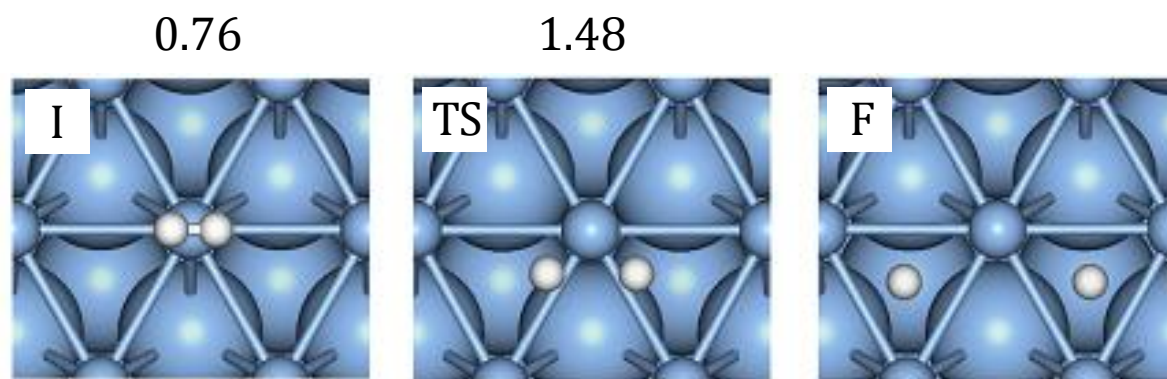


Figure S1. H₂ dissociation over Ag(111). The H-H distance is reported in Å.

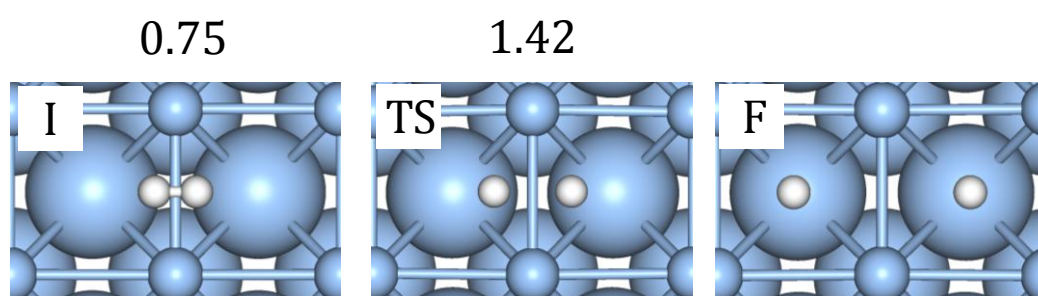


Figure S2. H₂ dissociation over Ag(100). The H-H distance is reported in Å.

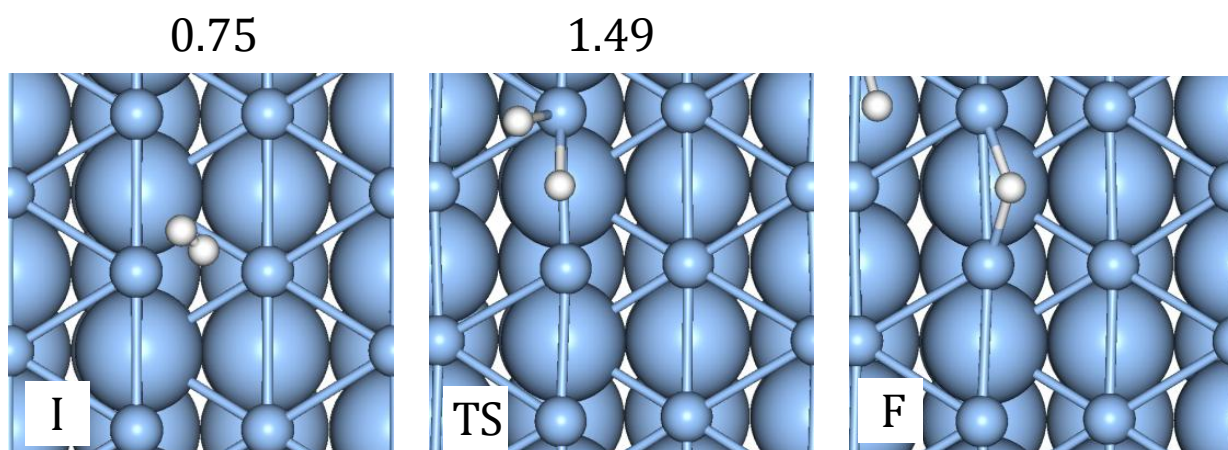


Figure S3. H₂ dissociation over Ag(211). The H-H distance is reported in Å.

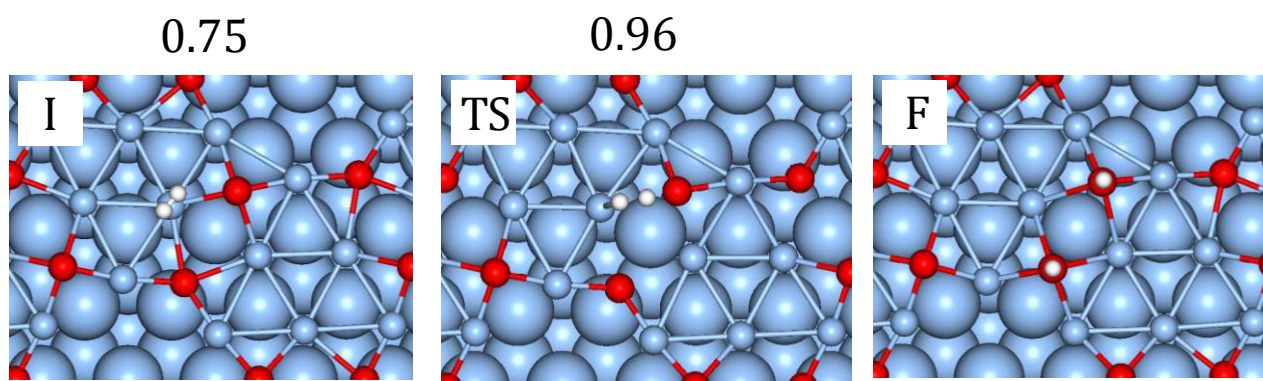


Figure S4. H₂ dissociation over *p*(4x4). The H-H distance is reported in Å. Note that the barrier for H₂ dissociation is related to H diffusion over the surface, hence the H-H distance is long in the TS. The H-H distance is reported in Å.

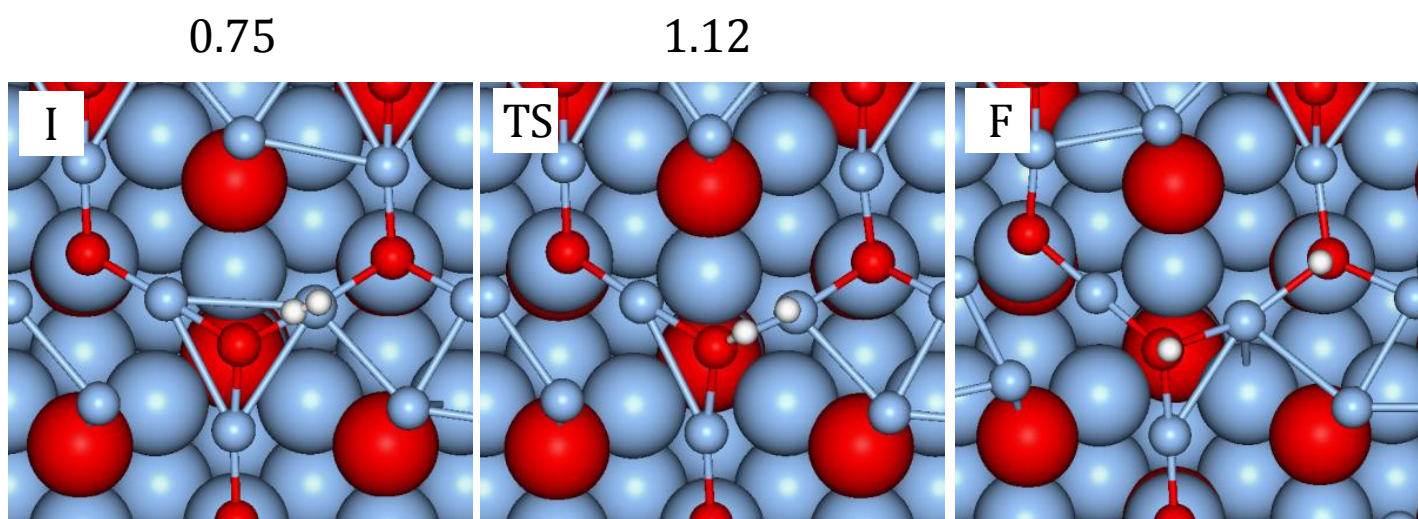


Figure S5. H₂ dissociation over Ag₂O(111). In the final state (F) formation of two OH groups is observed. The H-H distance is reported in Å.

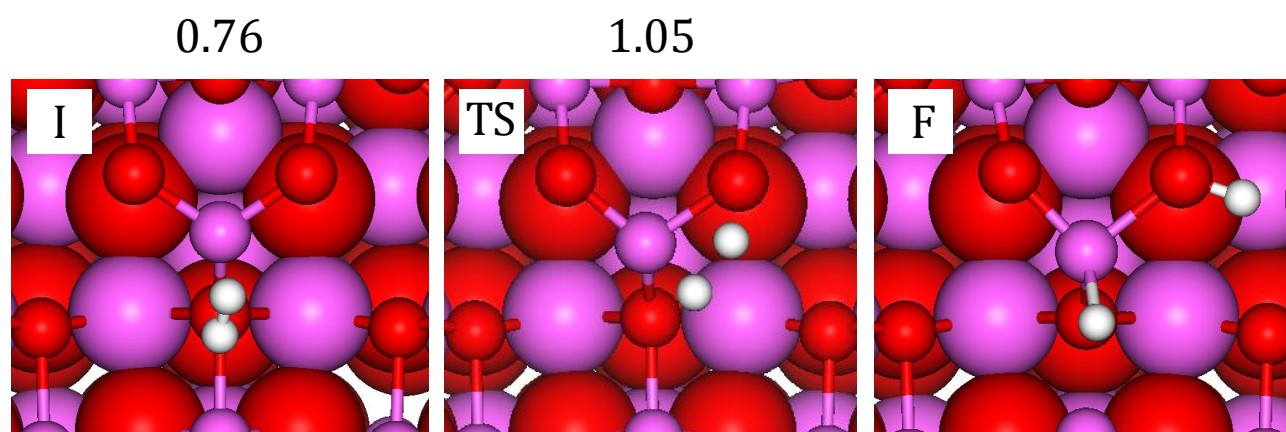


Figure S6. H₂ dissociation over Al₂O₃(110). In the initial state (I), the H₂ molecule is adsorbed over the Al_{III} site. Upon dissociation (F) electron pairing leads to formation of an Ag-H and O-H pair. The H-H distance is reported in Å.

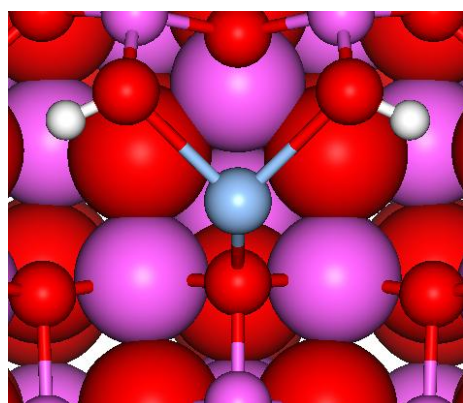


Figure S7. The final state for dissociated H₂ over Ag@Al₂O₃(110)-b.

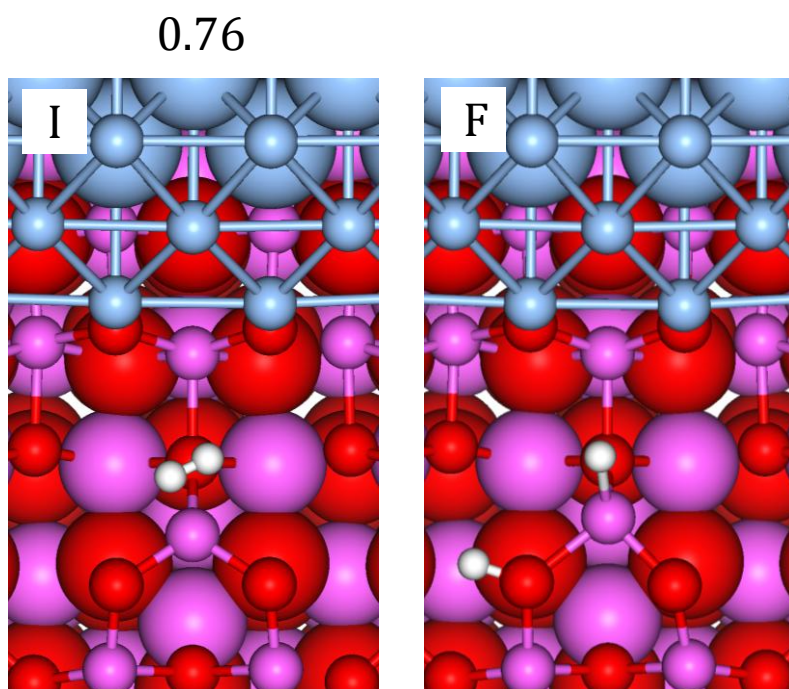


Figure S8. Top view of molecular and dissociated H₂ adsorption over Ag_{NPM}/Al₂O₃(110). Molecular adsorption occurs over the Al_{III} site and upon dissociation an Al-H and O-H pair is formed owing to electron pairing.

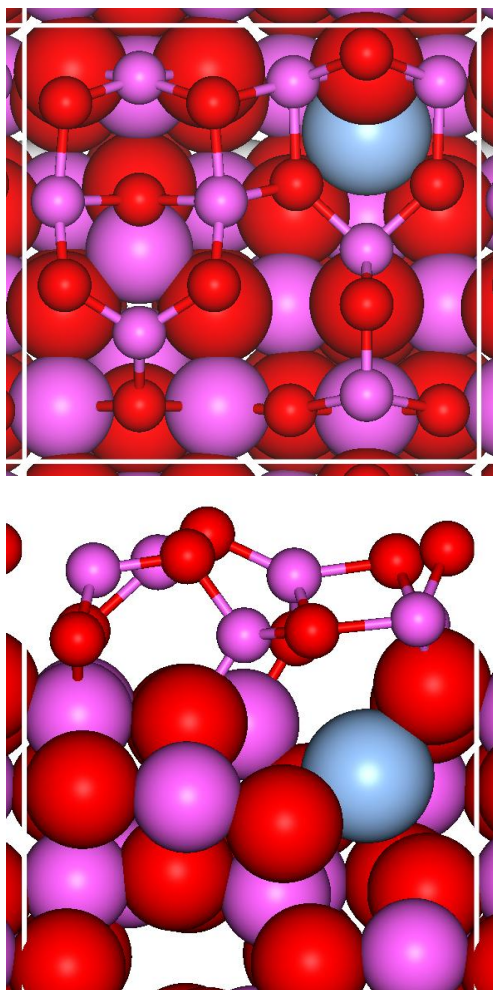


Figure S9. Top and side view of Ag@Al₂O₃(110)-a.