Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Activity of Faujasite Supported Gold Monomer towards Water Gas Shift Reaction: Hybrid Density Functional Theory/Molecular Mechanics Approach

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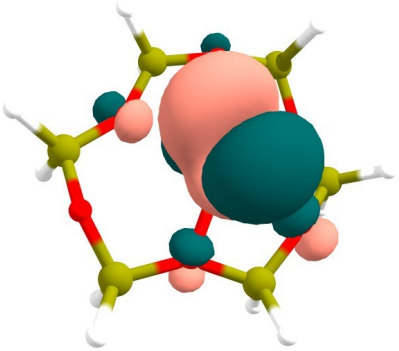
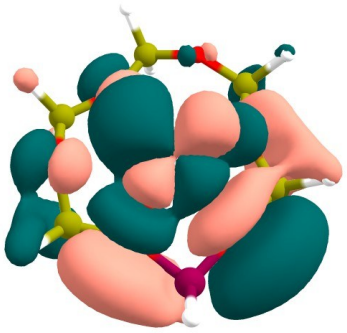
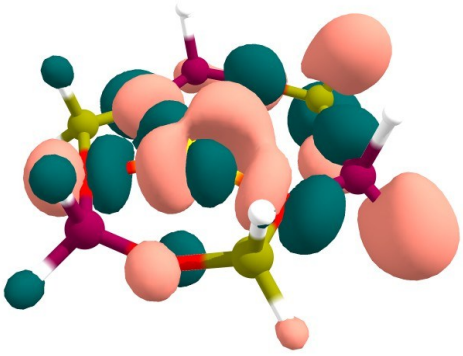


(a) Au^0 /FAU, HOMO-2

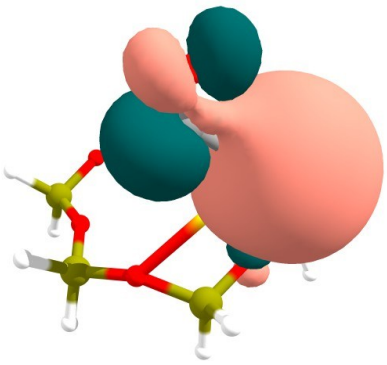


(b) Au^+ /FAU, HOMO-1

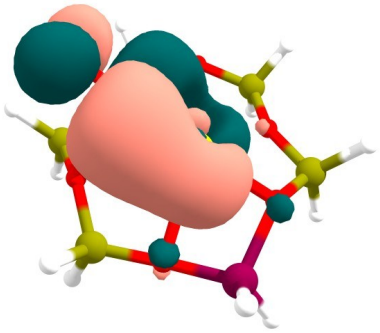


(c) Au^{3+} /FAU, HOMO-2

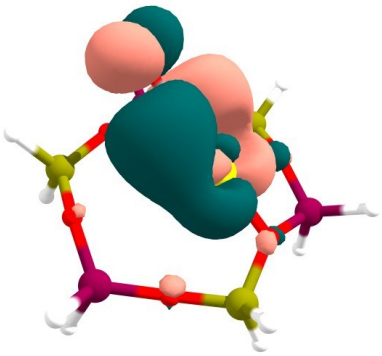
Figure S1: Frontier orbitals illustrating the interaction between Au and the zeolite O atoms in Au^n/FAU, n=0, +1 and +3.



(a) Au^0-CO/FAU, HOMO

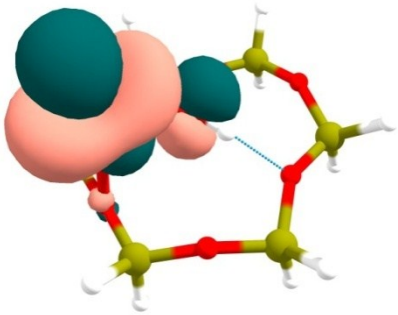


(b) Au^+-CO/FAU, LUMO

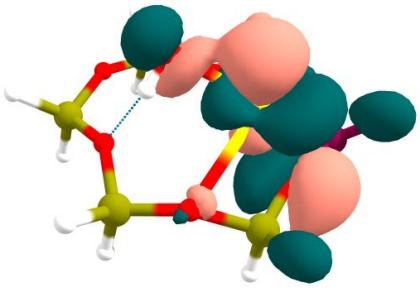


(c) Au^{3+}-CO/FAU, LUMO+1

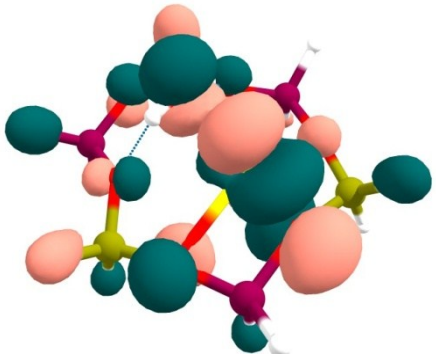
Figure S2: Frontier orbitals illustrating the interaction between CO and the faujasite supported Au centre in the CO adsorbed complexes of Au^n/FAU, n=0, +1 and +3.



(a) Au^0-H_2O/FAU, HOMO-3



(b) Au^+-H_2O/FAU, HOMO-2



(c) Au^{3+}-H_2O/FAU, HOMO-4

Figure S3: Frontier orbitals illustrating the interaction between H_2O and the faujasite supported Au centre in the H_2O adsorbed complexes of Au^n/FAU, n=0, +1 and +3.

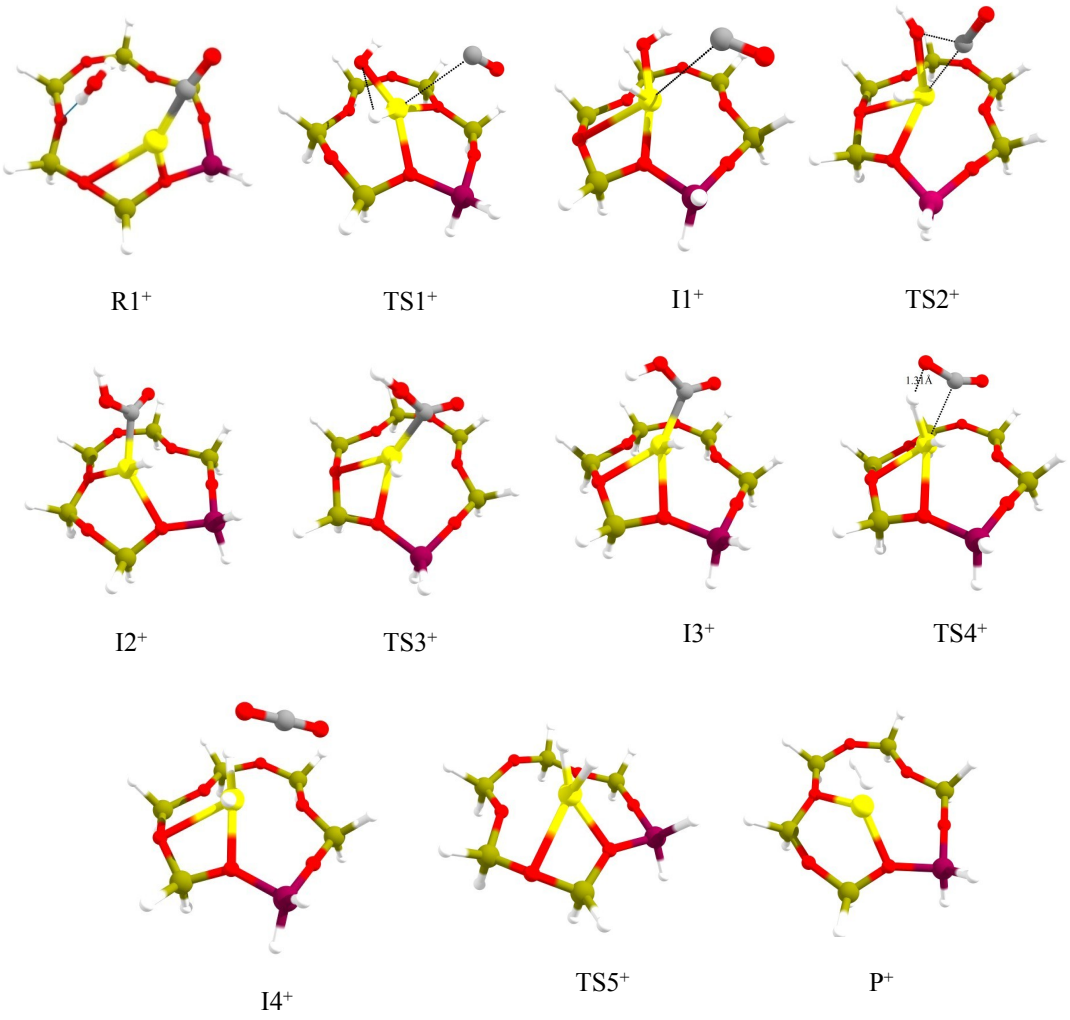


Figure S4: Structures of various intermediates and transition states observed during the reaction on Au^{+}/FAU.

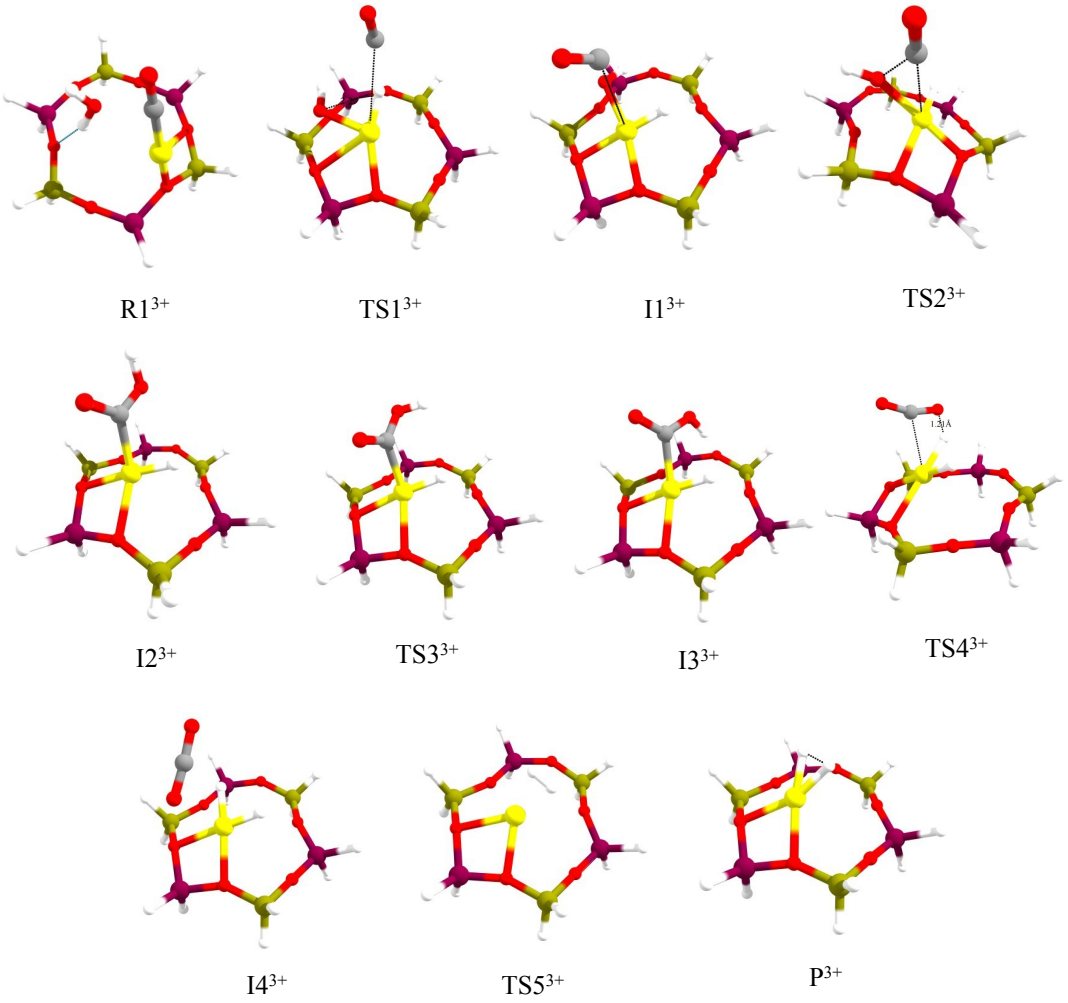


Figure S5: Structures of various intermediates and transition states observed during the reaction on Au^{3+}/FAU.