supporting information for

CO_2 reduction on metal-doped SnO_2(110) surface catalysts: manipulating the product by changing the ratio of Sn:O

Lei Cui,[1,2] DaDi Zhang,[2,*] Yuan Kong,[1,†] and Xiao Zheng[1]

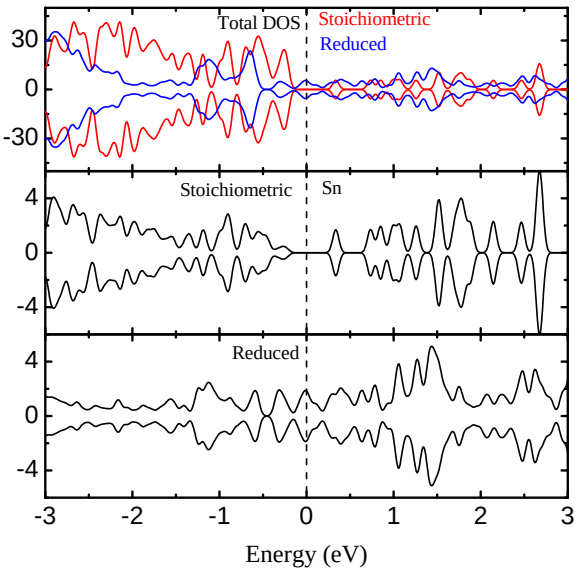
[1] *Department of Chemical Physics and Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, China*

[2] *National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China*

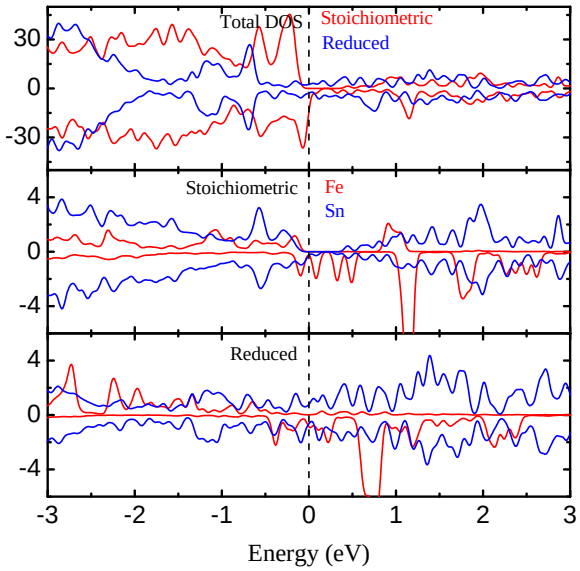
(Dated: May 10, 2021)

RESULTS OF OTHER METALS

The results of the PDOS for the catalytic active sites of SnO_2 (110) doped by Fe, Co,Cu, Ni, Ru, Rh, Ag, Pd, Ir, Os, Pt, and Au are shown in SI.1.

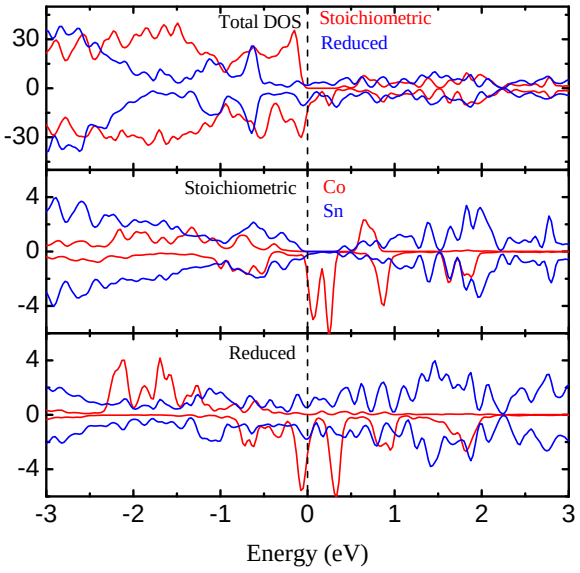


SI.1.Total and partral density of states for the catalytic active site of reduced (red) and stoichiometric (blue) SnO_2 (110). Fermi level is represented by a dotted line.

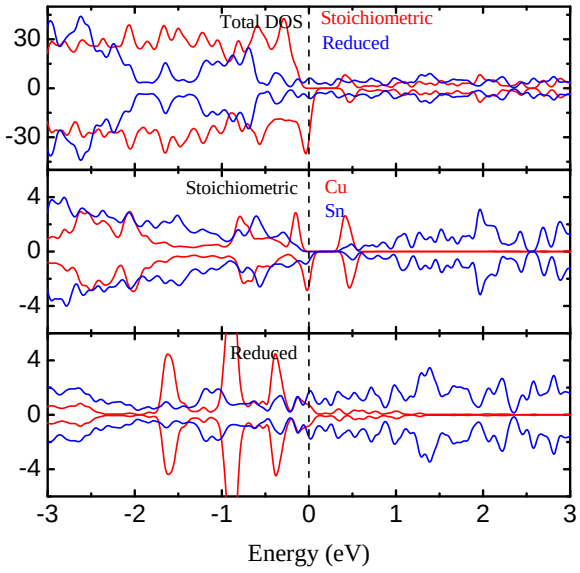


SI.2. Total and partral density of states for the catalytic active site of reduced and stoichiometric Fe-doped SnO_2 (110). Fermi level is represented by a dotted line.

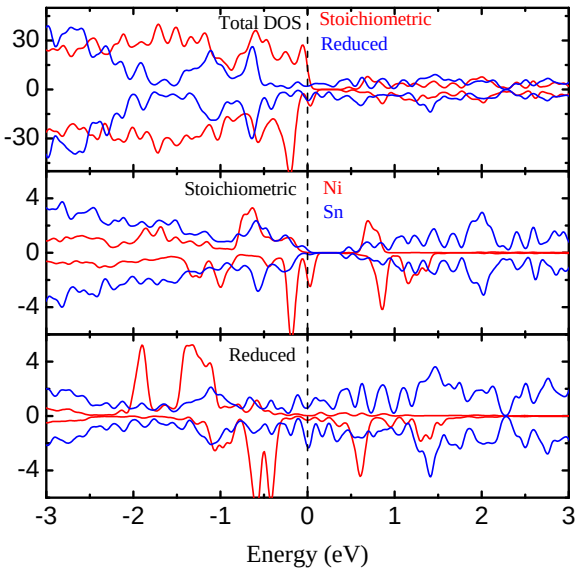
* zhangdadi@ustc.edu.cn
† kongyuan@ustc.edu.cn



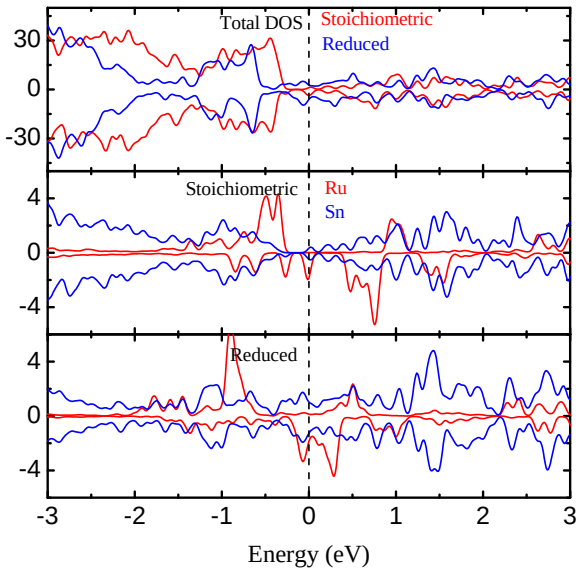
SI.3. Total and partral density of states for the catalytic active site of reduced and stoichiometric Co-doped SnO_2 (110). Fermi level is represented by a dotted line.



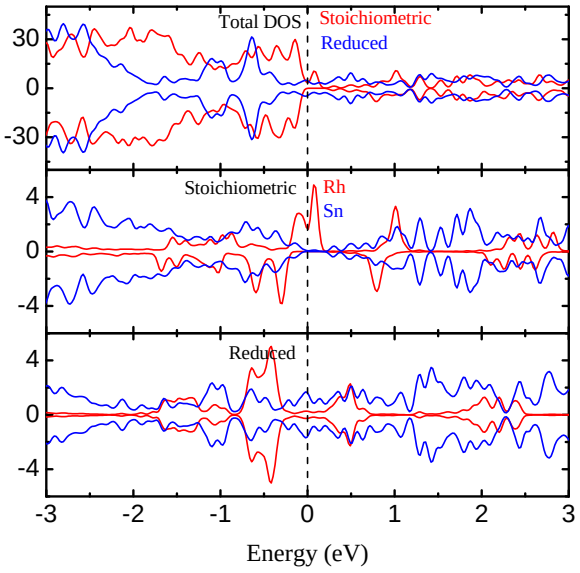
SI.5. Total and partral density of states for the catalytic active site of reduced and stoichiometric Cu-doped SnO_2 (110). Fermi level is represented by a dotted line.



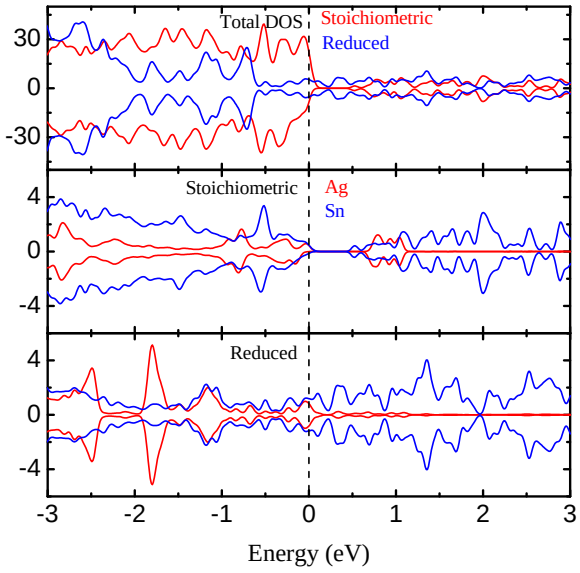
SI.4. Total and partral density of states for the catalytic active site of reduced and stoichiometric Ni-doped SnO_2 (110). Fermi level is represented by a dotted line.



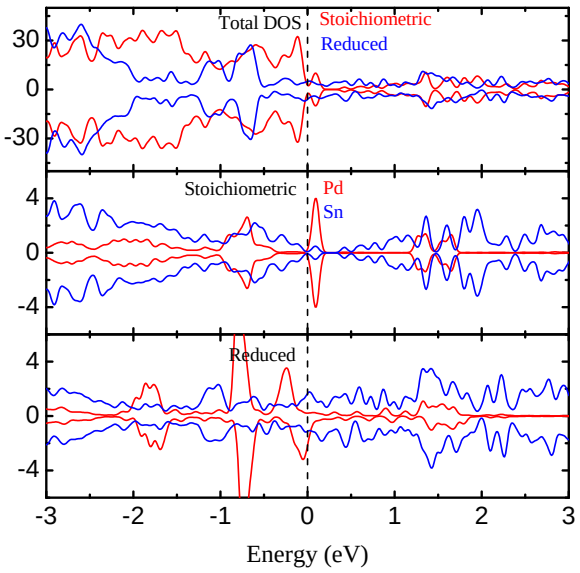
SI.6. Total and partral density of states for the catalytic active site of reduced and stoichiometric Ru-doped SnO_2 (110). Fermi level is represented by a dotted line.



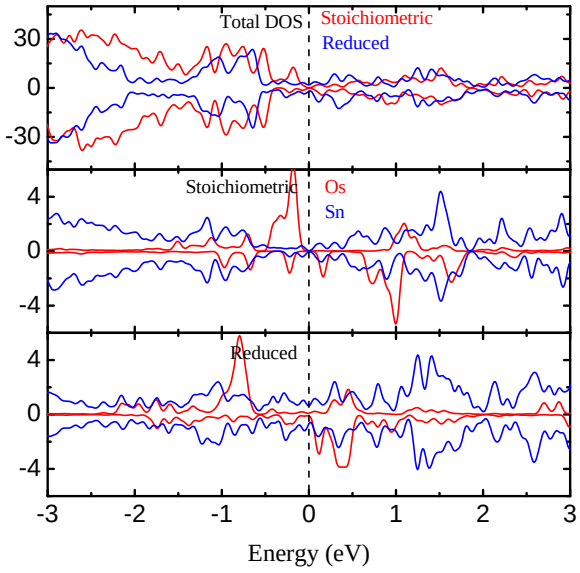
SI.7. Total and partral density of states for the catalytic active site of reduced and stoichiometric Rh-doped SnO_2 (110). Fermi level is represented by a dotted line.



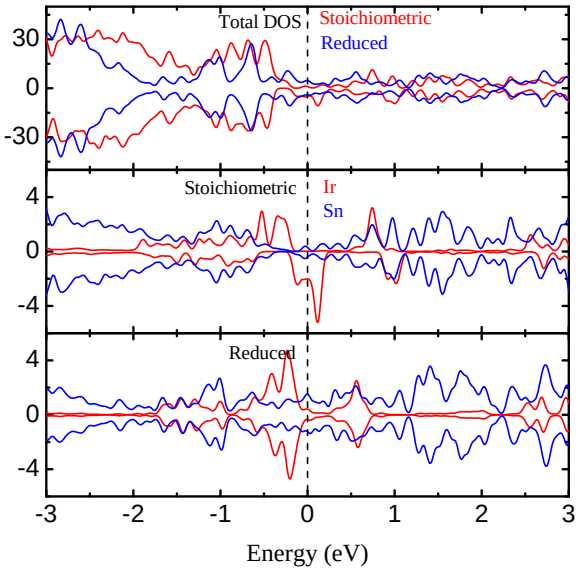
SI.9. Total and partral density of states for the catalytic active site of reduced and stoichiometric Ag-doped SnO_2 (110). Fermi level is represented by a dotted line.



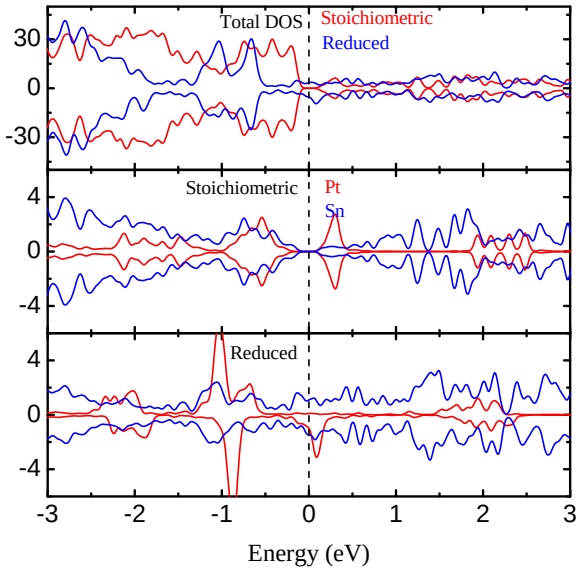
SI.8. Total and partral density of states for the catalytic active site of reduced and stoichiometric Pd-doped SnO_2 (110). Fermi level is represented by a dotted line.



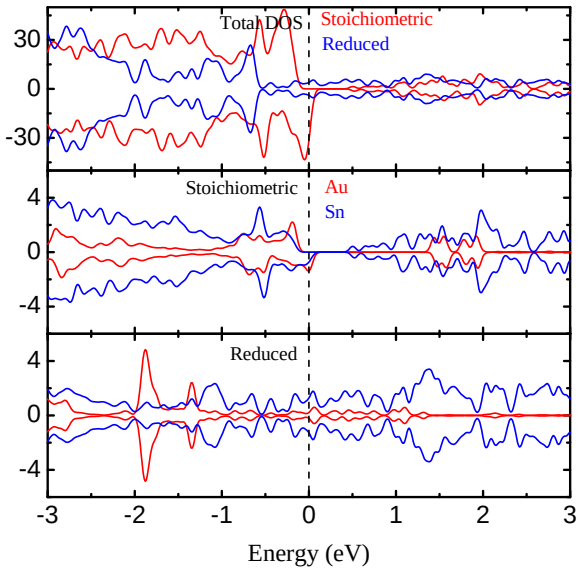
SI.10. Total and partral density of states for the catalytic active site of reduced and stoichiometric Os-doped SnO_2 (110). Fermi level is represented by a dotted line.



SI.11. Total and partral density of states for the catalytic active site of reduced and stoichiometric Ir-doped SnO_2 (110). Fermi level is represented by a dotted line.

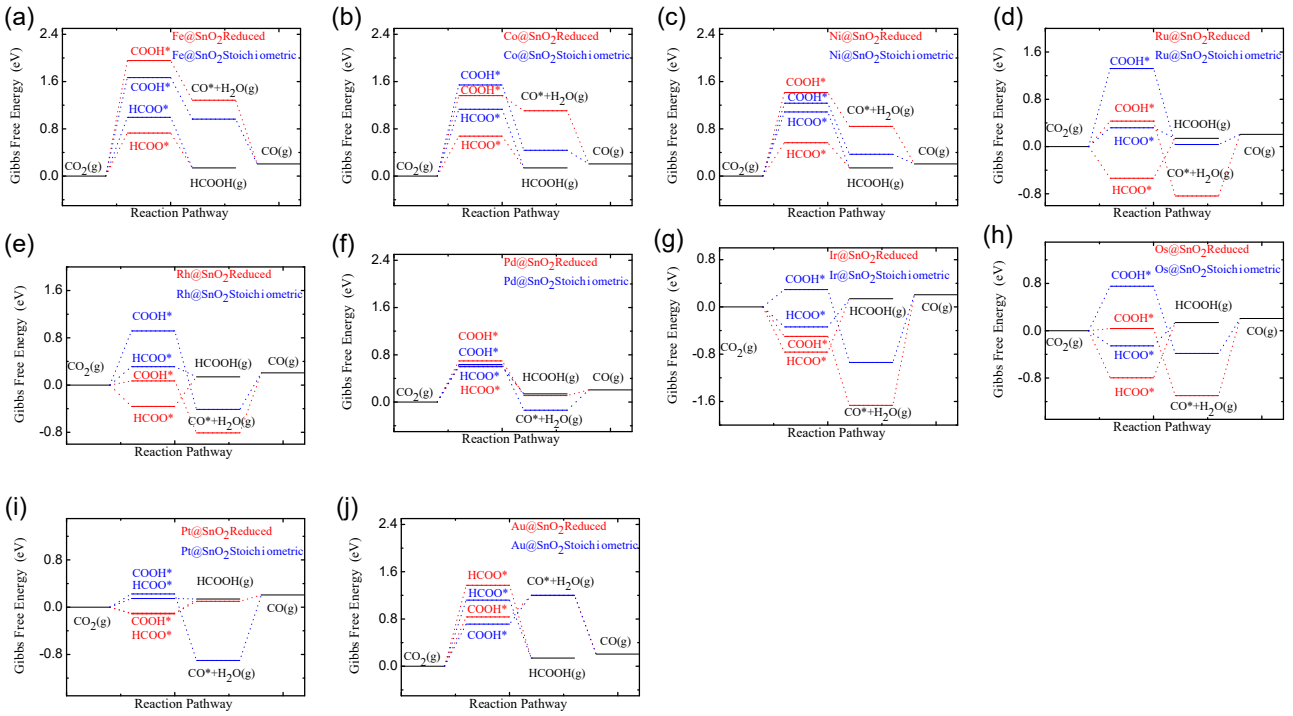


SI.12. Total and partral density of states for the catalytic active site of reduced and stoichiometric Pt-doped SnO_2 (110). Fermi level is represented by a dotted line.

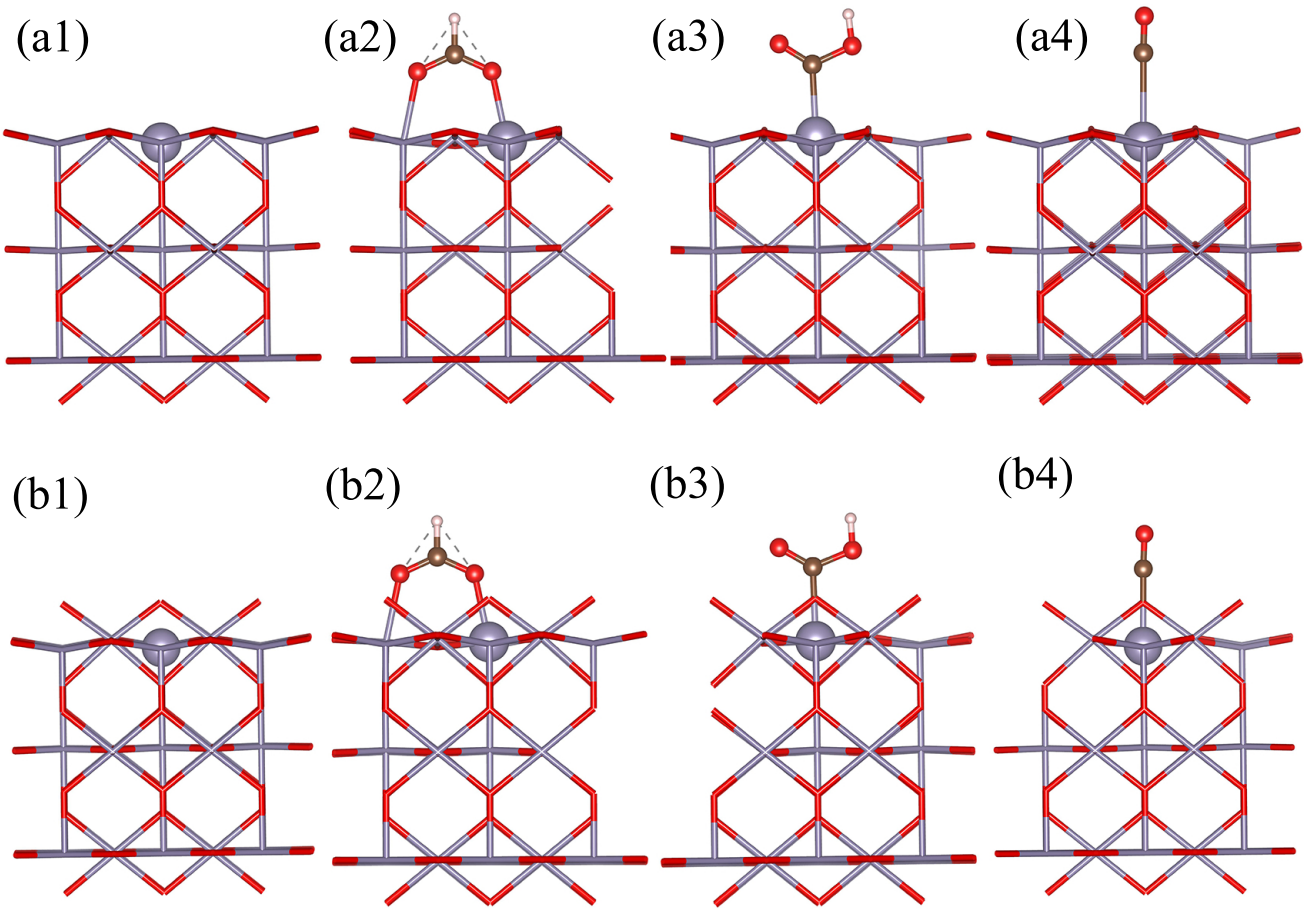


SI.13. Total and partral density of states for the catalytic active site of reduced and stoichiometric Au-doped SnO_2 (110). Fermi level is represented by a dotted line.

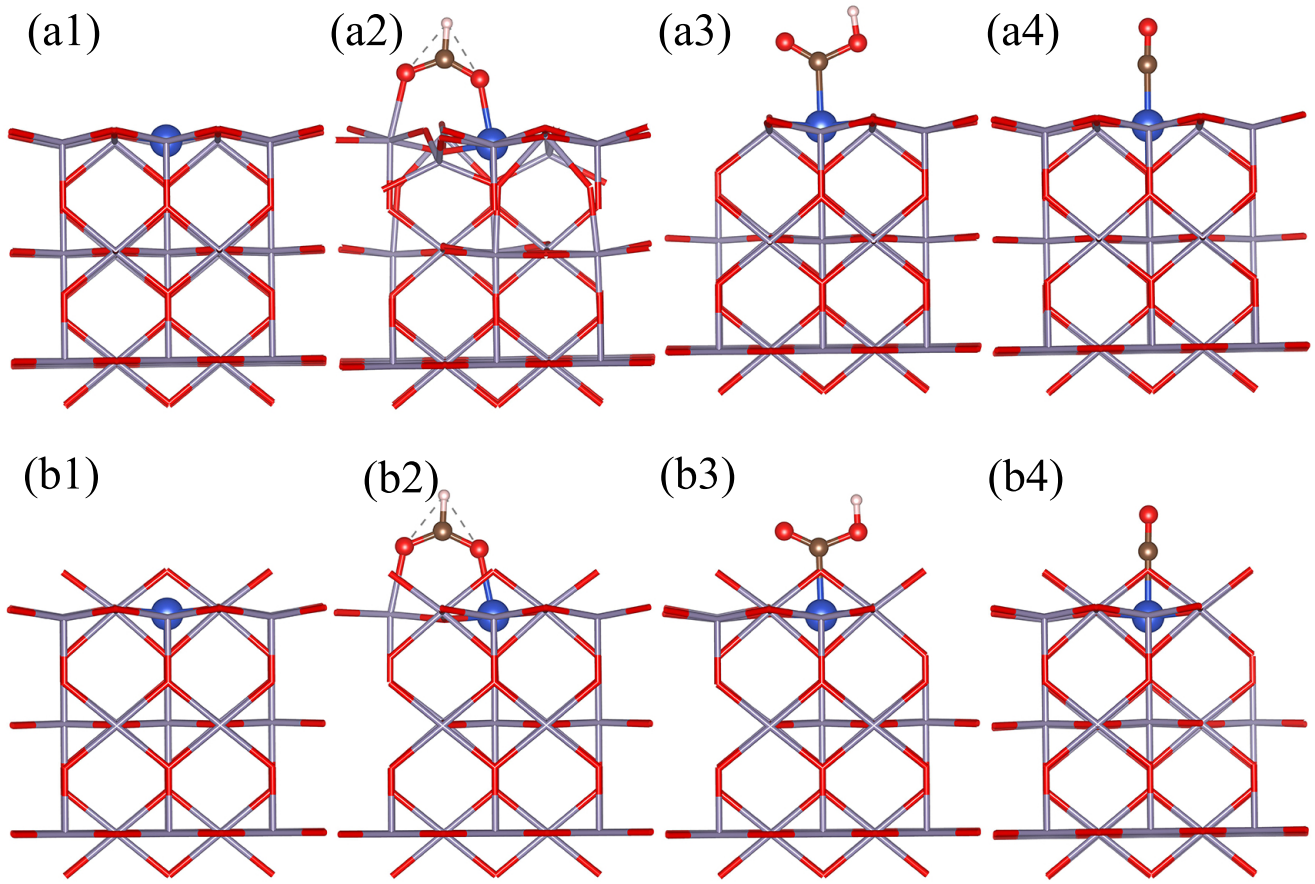
The results of SnO_2 (110) doped with Fe, Co, Ni, Ru, Rh, Pd, Ir, Os, Pt, and Au are shown in SI.14. The side views of CO_2RR's intermediate state with non-doped SnO_2 (110) are shown in SI.15. The side views of CO_2RR's intermediate state with metal-doped SnO_2 (110) are shown in SI.16.



SI.14. Reaction paths and free energy of reduced (red) and stoichiometric (blue) SnO_2 (110): (a) Fe@SnO_2 (110), (b) Co@SnO_2 (110), (c) Ni@SnO_2 (110), (d) Ru@SnO_2 (110), (e) Rh@SnO_2 (110), (f) Pd@SnO_2 (110), (g) Au@SnO_2 (110), (h) Ir@SnO_2 (110), (i) Os@SnO_2 (110), (j) Pt@SnO_2 (110).



SI.15. Side views of reduced (a1) SnO_2 (110), (a2) HCOO*SnO_2 (110), (a3) COOH*SnO_2 (110), (a4) CO*SnO_2 (110), and stoichiometric (b1) SnO_2 (110), (b2) HCOO*SnO_2 (110), (b3) COOH*SnO_2 (110), (b4) CO*SnO_2 (110). The red, gray, brown, white balls represent O, Sn, C, H atoms, respectively.



SI.16. Side views of reduced (a1) metal(X)-doped SnO_2 (110), (a2) HCOO*X@SnO_2 (110), (a3) COOH*X@SnO_2 (110), (a4) CO*X@SnO_2 (110), and stoichiometric (b1) metal(X)-doped SnO_2 (110), (b2) HCOO*X@SnO_2 (110), (b3) COOH*X@SnO_2 (110), (b4) CO*X@SnO_2 (110). The red, gray, blue, brown, white balls represent O, Sn, metal, C, H atoms, respectively.