Electronic Supplementary Material (ESI) for Nanoscale.

Self-passivated Edges of ZnO Nanoribbon: A Global Search

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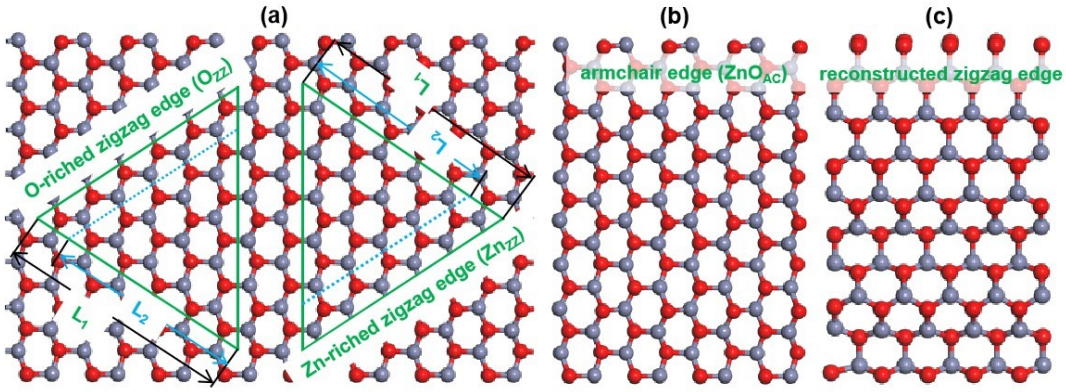

Fig. S1 The representative structures which can be used to calculate edge formation energy. (a) Pristine zigzag edges with Zn-rich and O-rich, (b) pristine armchair edges, (c) reconstructed zigzag edges.

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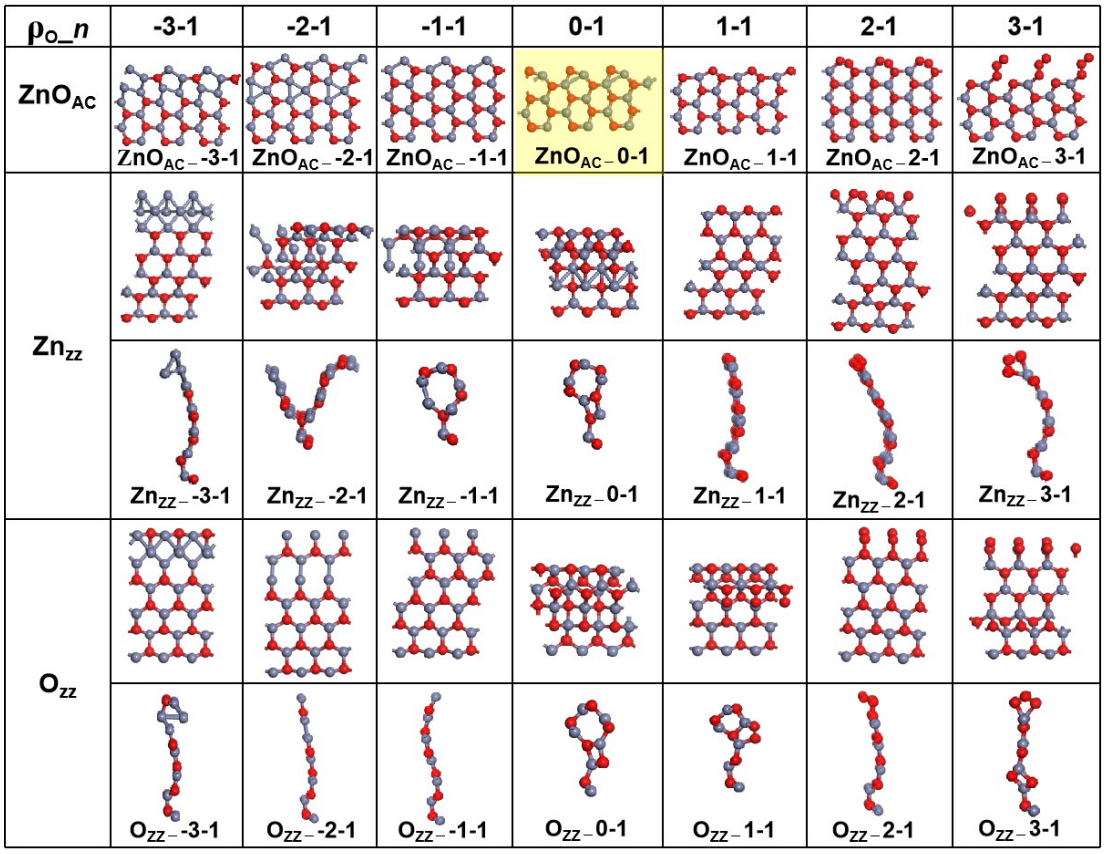

Fig. S2 Top and side views of the first low-lying reconstructed structures of the ZnO_{AC}, Zn_{ZZ} and O_{ZZ} edges at various different concentration of oxygen. The red and gray spheres represent oxygen and zinic atoms, respectively. The structure with yellow background can be obtained by slightly distorting pristine armchair edge.

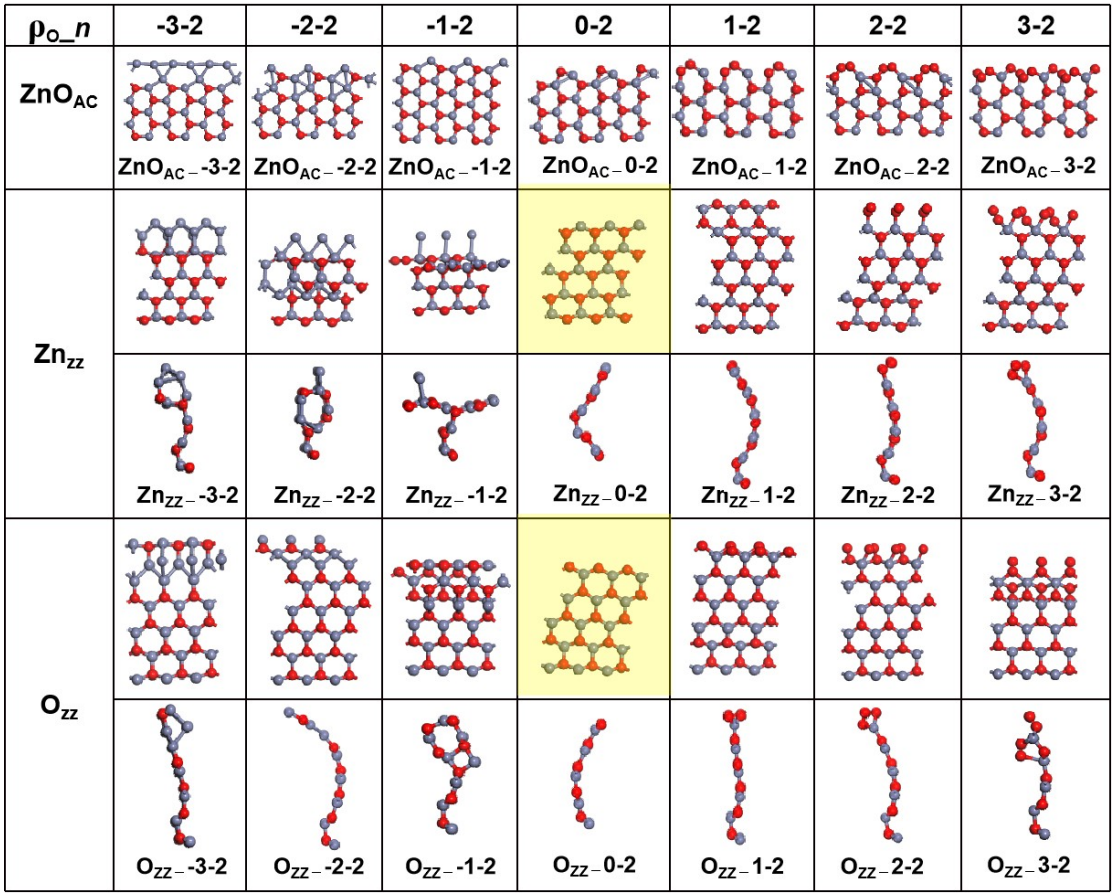

Fig. S3 Top and side views of the second low-lying reconstructed structures of the ZnO_{AC}, Zn_{ZZ} and O_{ZZ} edges at various different concentration of oxygen. The red and gray spheres represent oxygen and zinic atoms, respectively. The structures with yellow background are pristine zigzag edges.

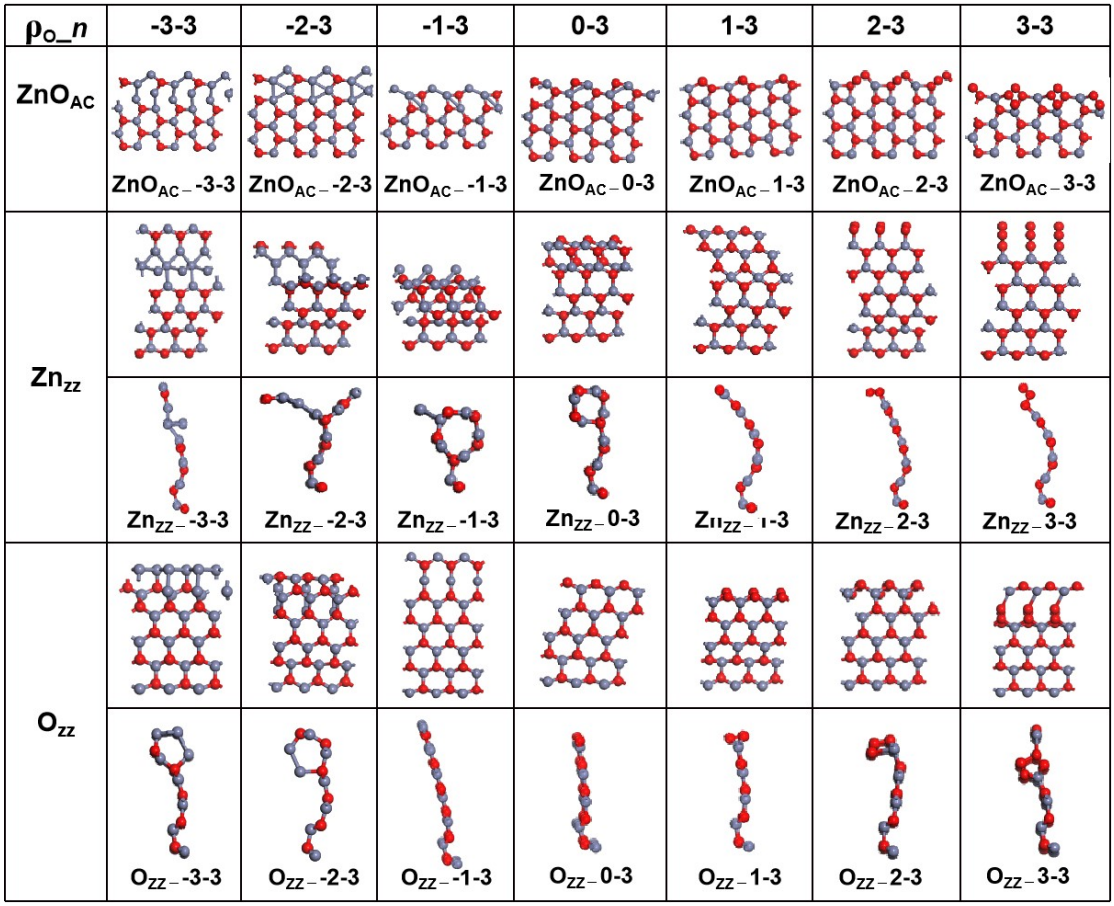

Fig. S4 Top and side views of the third low-lying edge reconstructed structures of the ZnO_{AC}, Zn_{ZZ} and O_{ZZ} edges at various different concentration of oxygen. The red and gray spheres represent oxygen and zinic atoms, respectively.

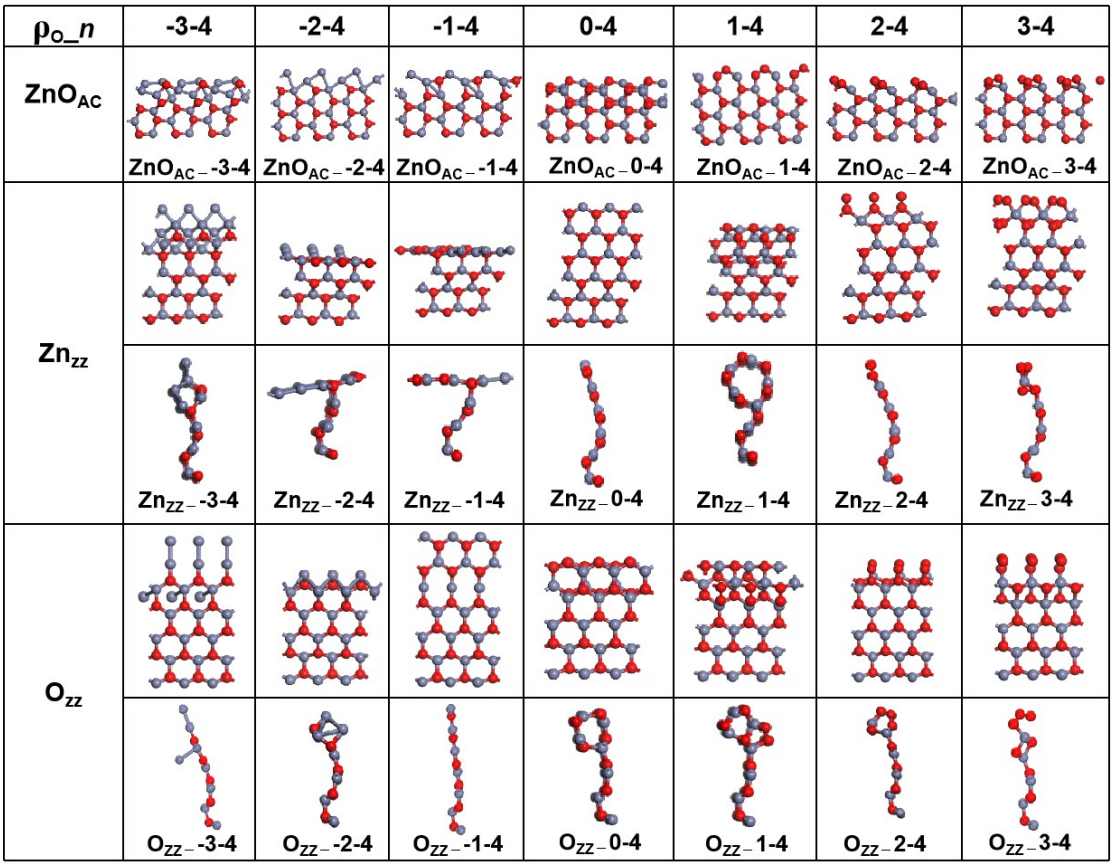

Fig. S5 Top and side views of the fourth low-lying reconstructed structures of the ZnO_{AC}, Zn_{ZZ} and O_{ZZ} edges at various different concentration of oxygen. The red and gray spheres represent oxygen and zinic atoms, respectively.

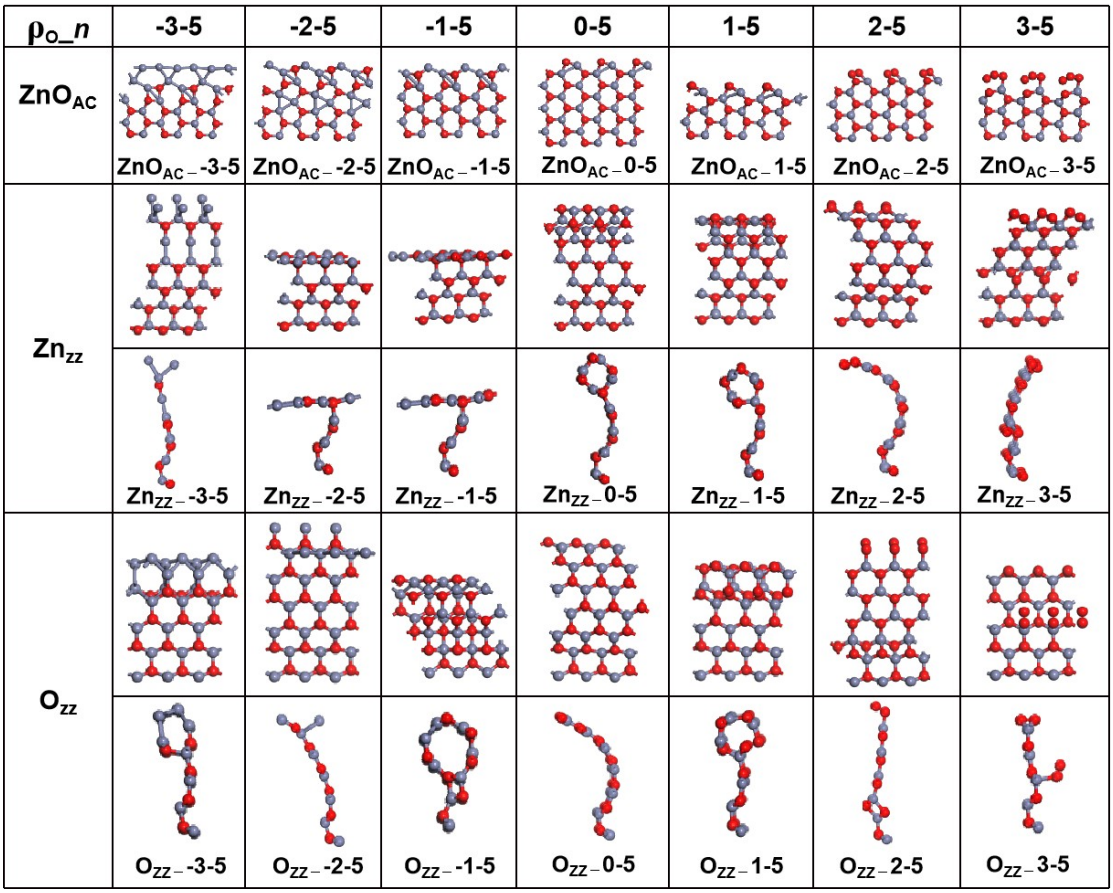

Fig. S6 Top and side views of the fifth low-lying reconstructed structures of the ZnO_{AC}, Zn_{ZZ} and O_{ZZ} edges at various different concentration of oxygen. The red and gray spheres represent oxygen and zinic atoms, respectively.

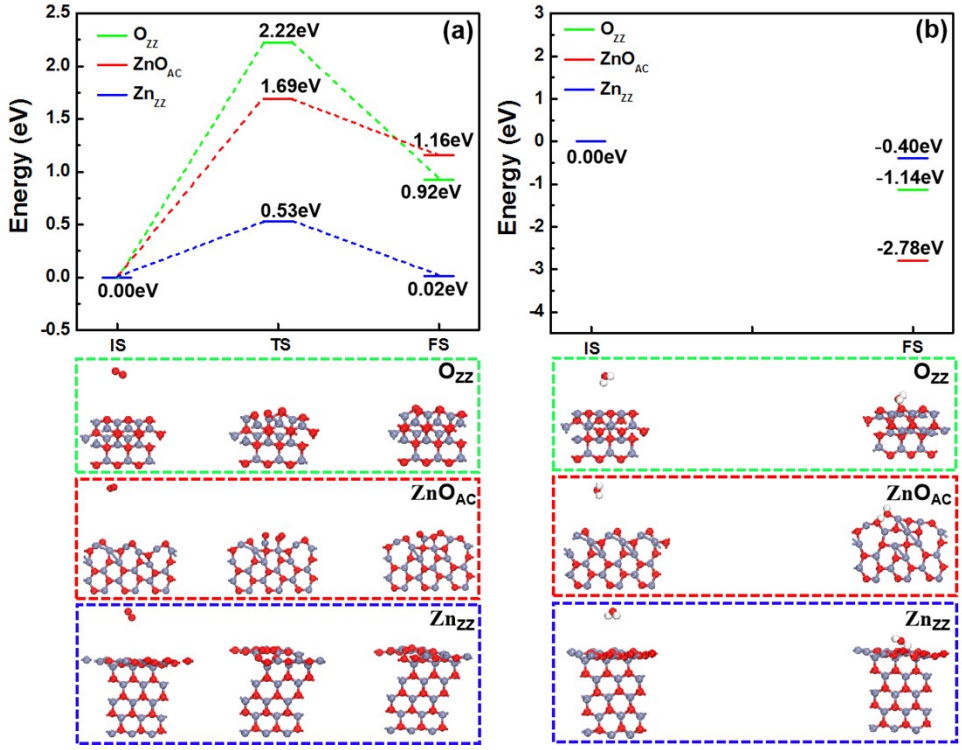

Fig. S7 The minimum energy reaction pathways for the dissociation of (a) O_2 and (b) H_2O molecules on three types of reconstructed edges (O_{ZZ}, ZnO_{AC} and Zn_{ZZ}), respectively. The red, gray and white balls represent oxygen, zinc and hydrogen atoms, respectively.

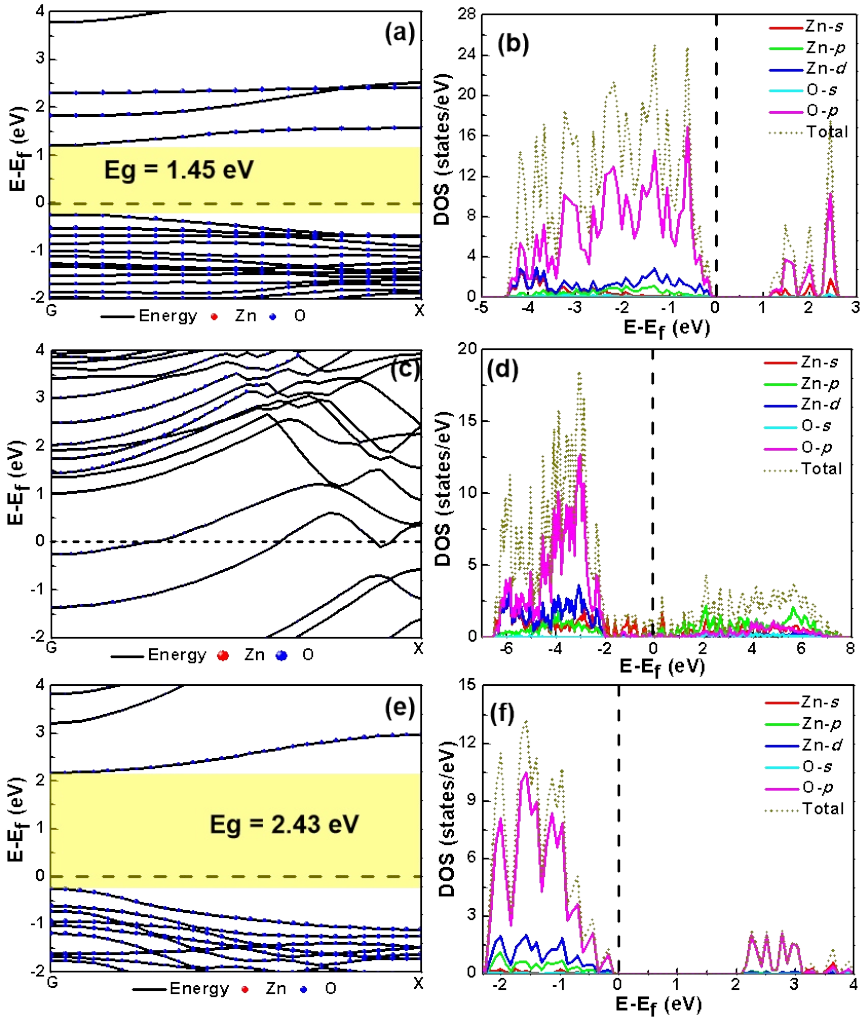

Fig. S8 The band structures and density of states (DOSs) of the other three stable edge reconstructed structures for (a, b) ZnO_{AC}, (c, d) Zn_{ZZ}, and (e, f) O_{ZZ} at the special concentration of oxygen.