

Supplementary Information

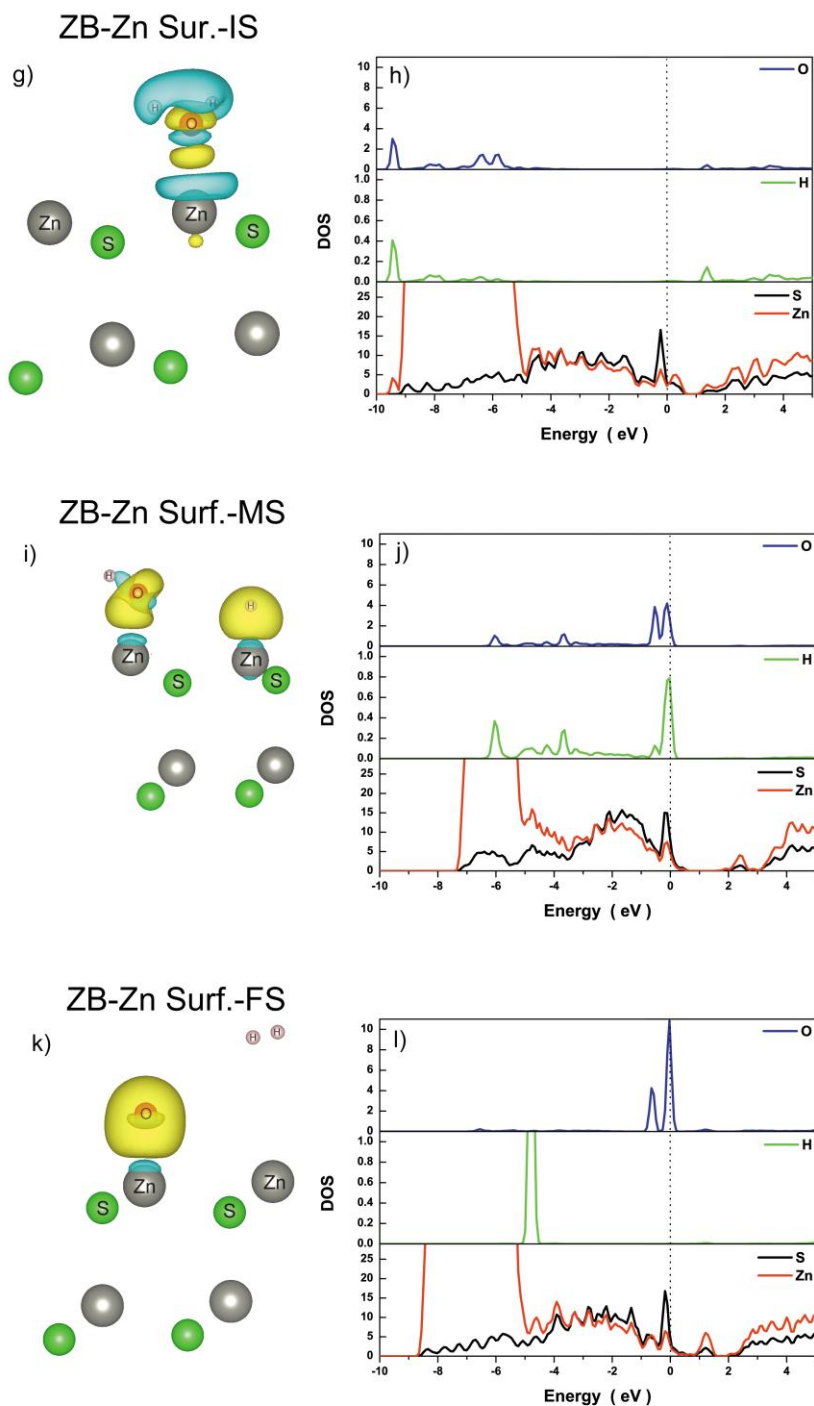


Figure 1S. Calculated DOSs and bonding charge density of states along the MEP path on the ZB (111) surface. *g*) and *h*) for IS, *i*) and *j*) for MS, and *k*) and *l*) for FS. Energies are referred to the Fermi level, which is marked by a vertical dash line.

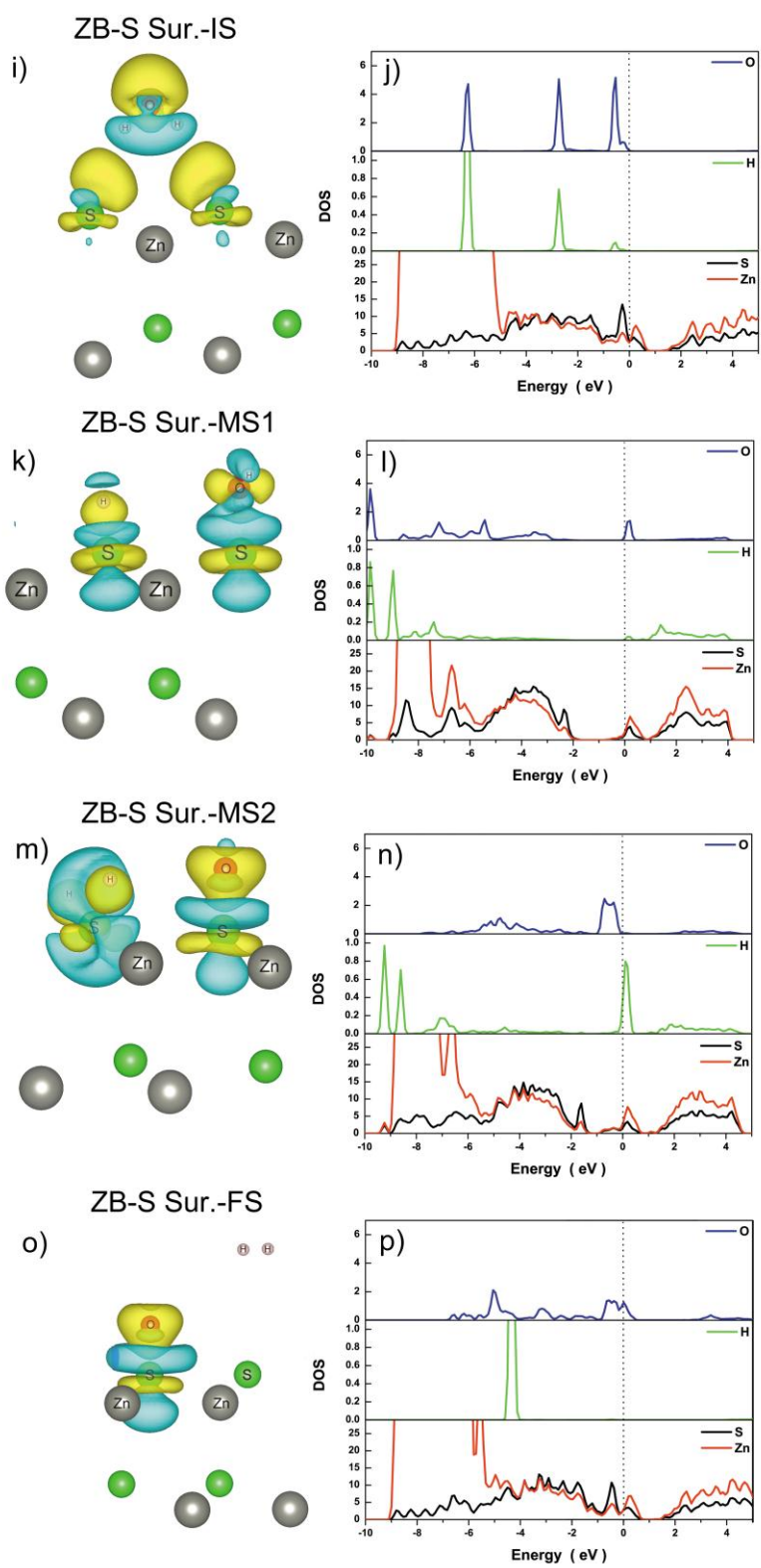


Figure 2S. Calculated DOSs and bonding charge density of states along the MEP path on the ZB (111) surface. *i*) and *j*) for IS, *k*) and *l*) for MS1, (*m*) and (*n*) for MS2, and *o*) and *p*) for FS. Energies are referred to the Fermi level, which is marked by a vertical dash line.

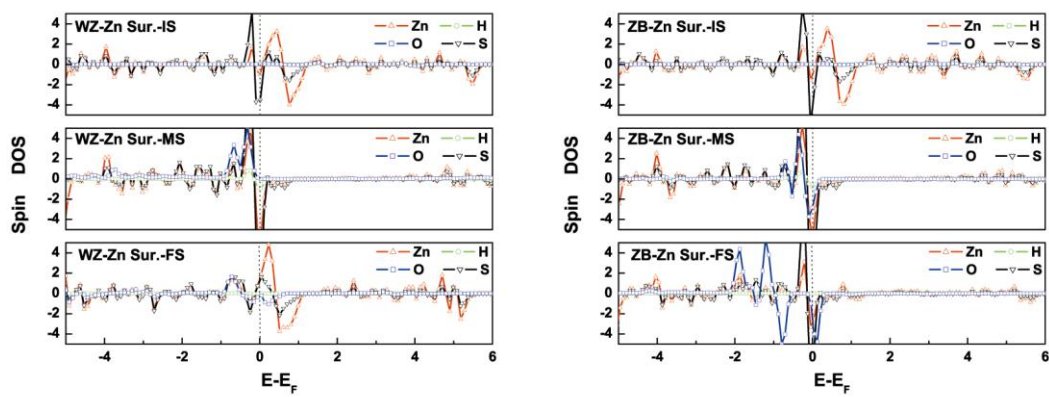


Figure 3S. Calculated Spin DOSs (Spin up minus Spin down) of states along the MEP path on the WZ (0001) and ZB (111) surfaces. Energies are referred to the Fermi level, which is marked by a vertical dash line.

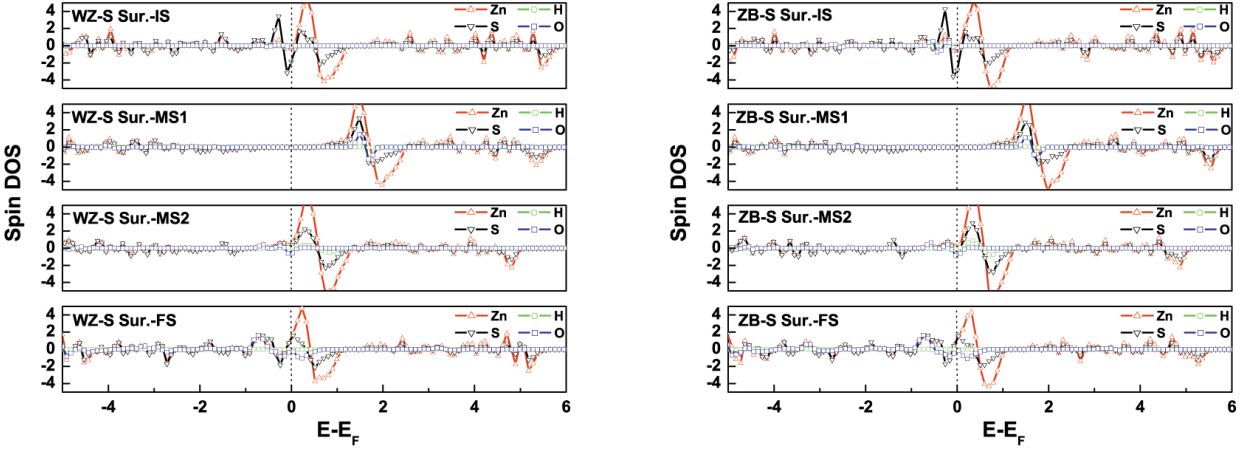


Figure 4S. Calculated Spin DOSs (Spin up minus Spin down) of states along the MEP path on the WZ (0001) and ZB (111) surfaces. Energies are referred to the Fermi level, which is marked by a vertical dash line.