Charge Transfer-Driven Modulation of Hydrogen Evolution Activity in NiCo LDHs via Main Group and 4d Metal Doping.

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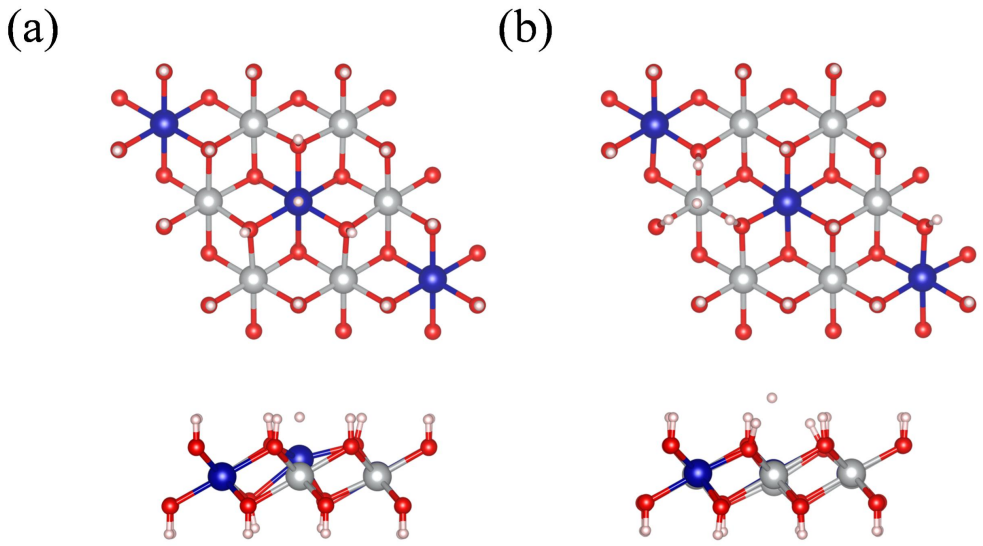

Figure S1. The optimized H adsorption configurations on (a) Co and (b) Ni sites in pristine NiCo LDHs.

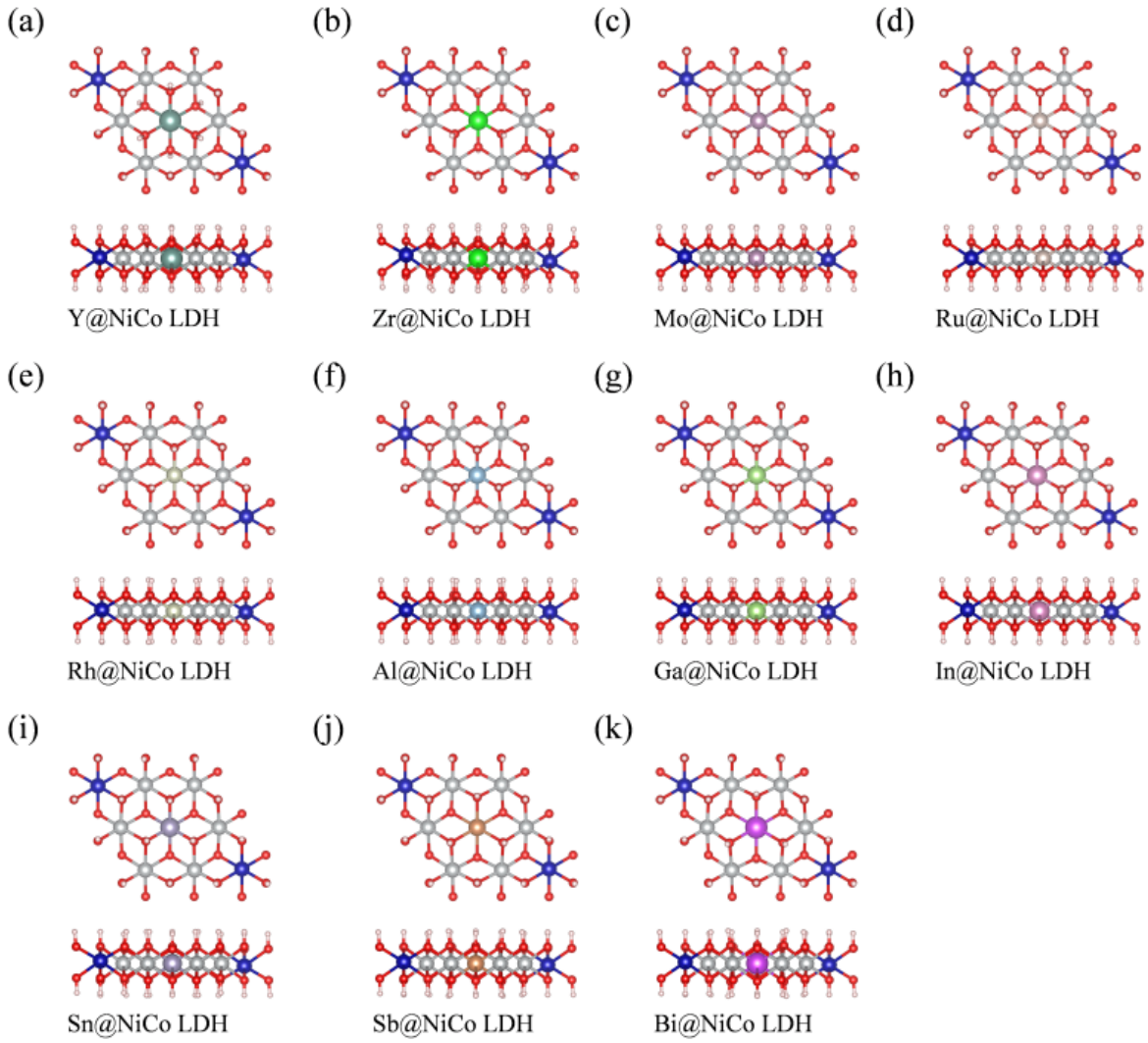

Figure S2. The optimized configurations of transition and main-group metal doped NiCo LDHs.

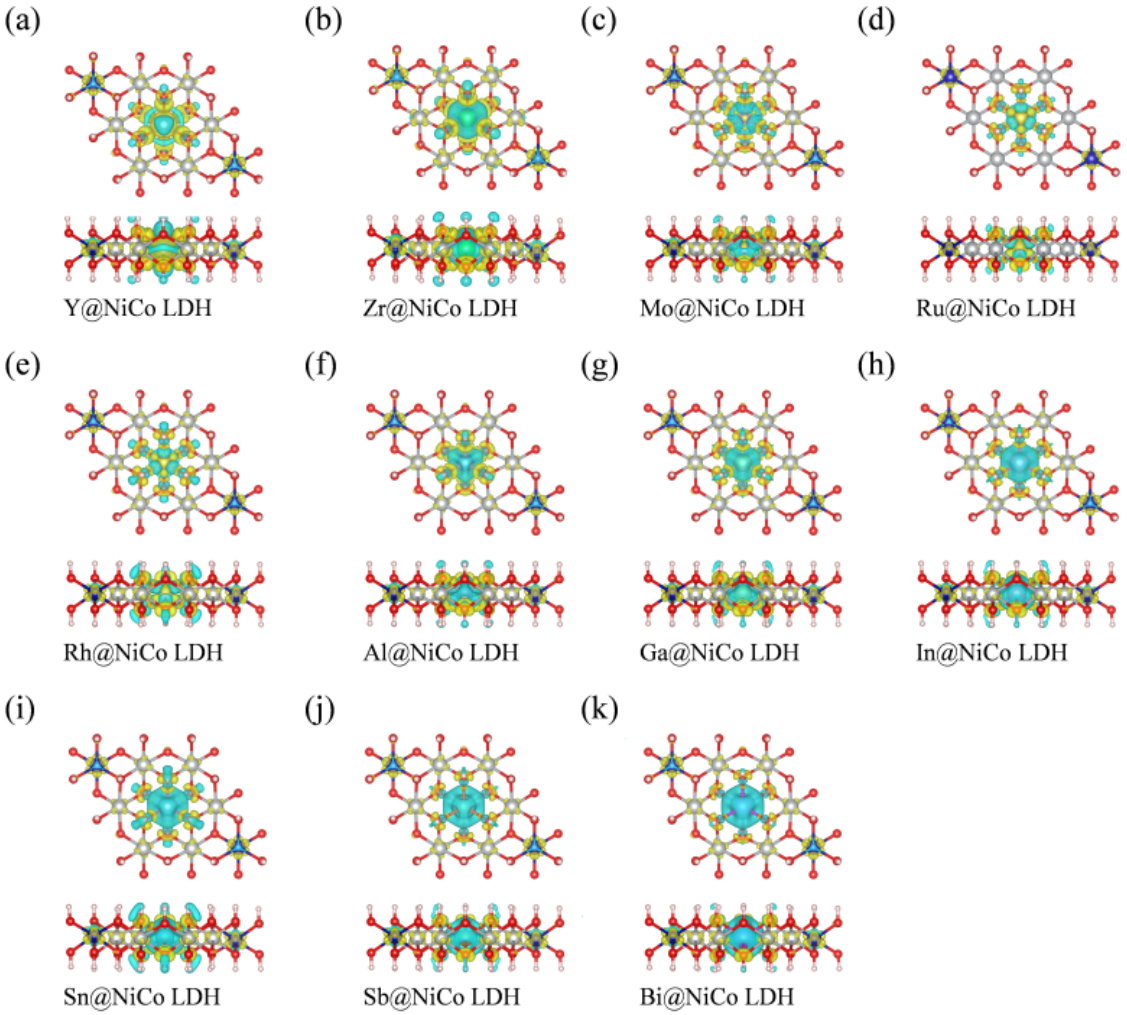

Figure S3. The charge density difference of metal doping configuration. The isosurface value is set to be 0.0065 *e*/bohr^3, the yellow region represents charge accumulation, and blue region denote charge depletion.

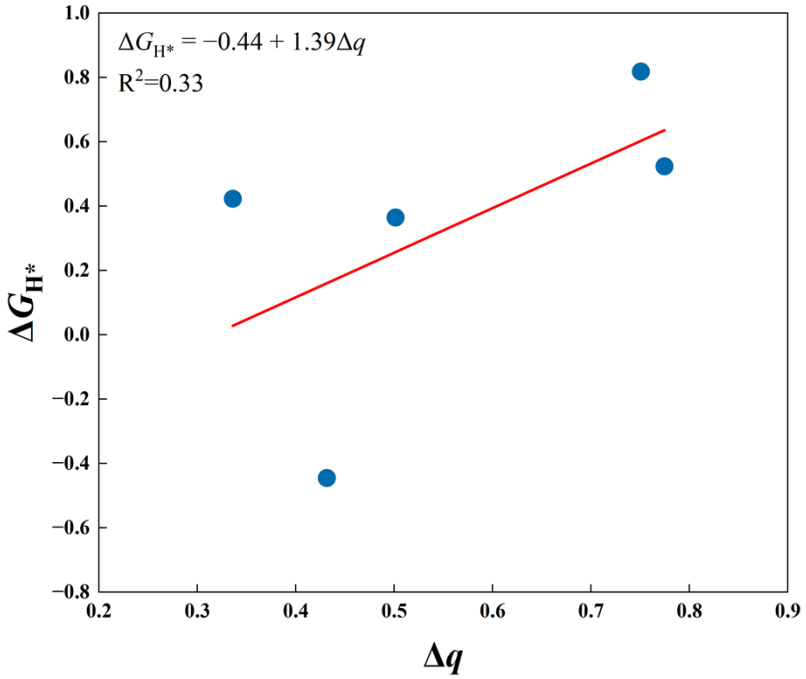

Figure S4. The correlation of Δq and ΔG_{H^*} for 4d transition metal-doped systems.

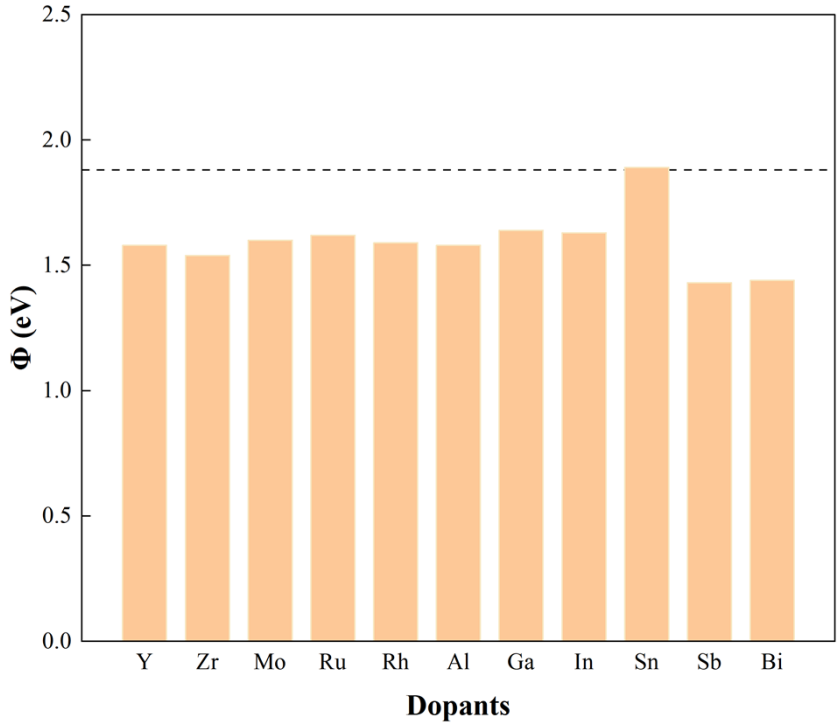

Figure S5. Work function of metal doped NiCo LDHs.

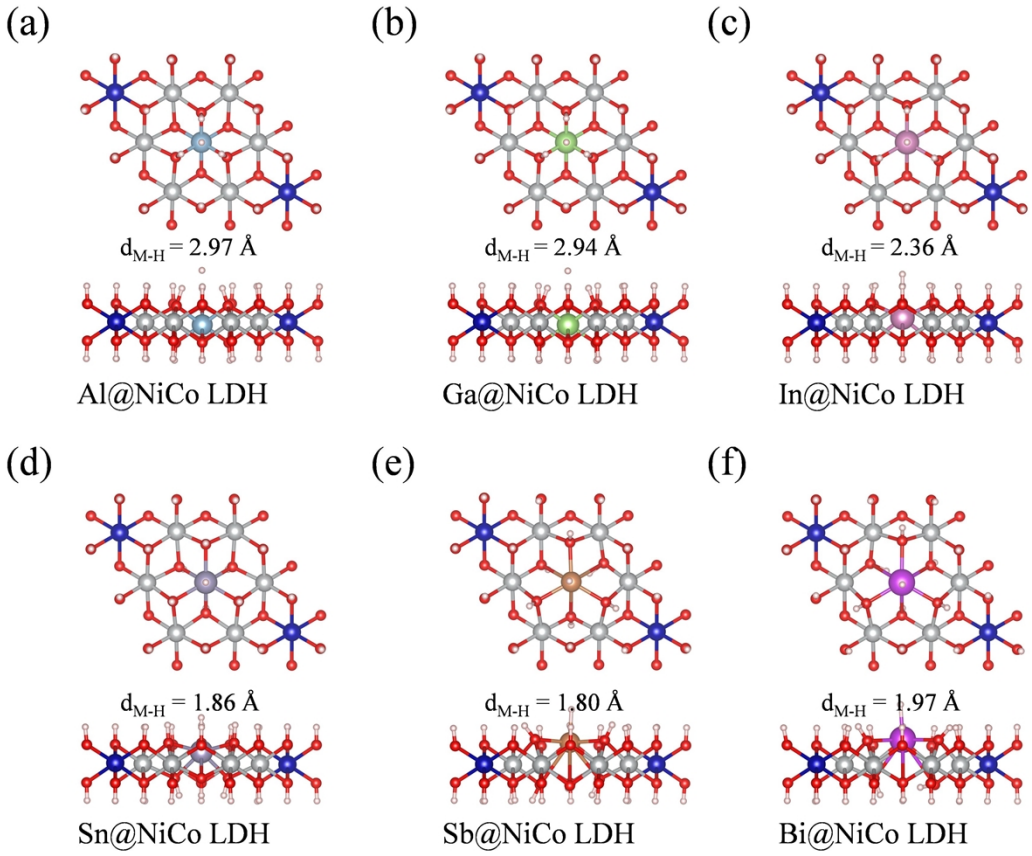

Figure S6. H adsorption configurations of main-group metal-doped systems.

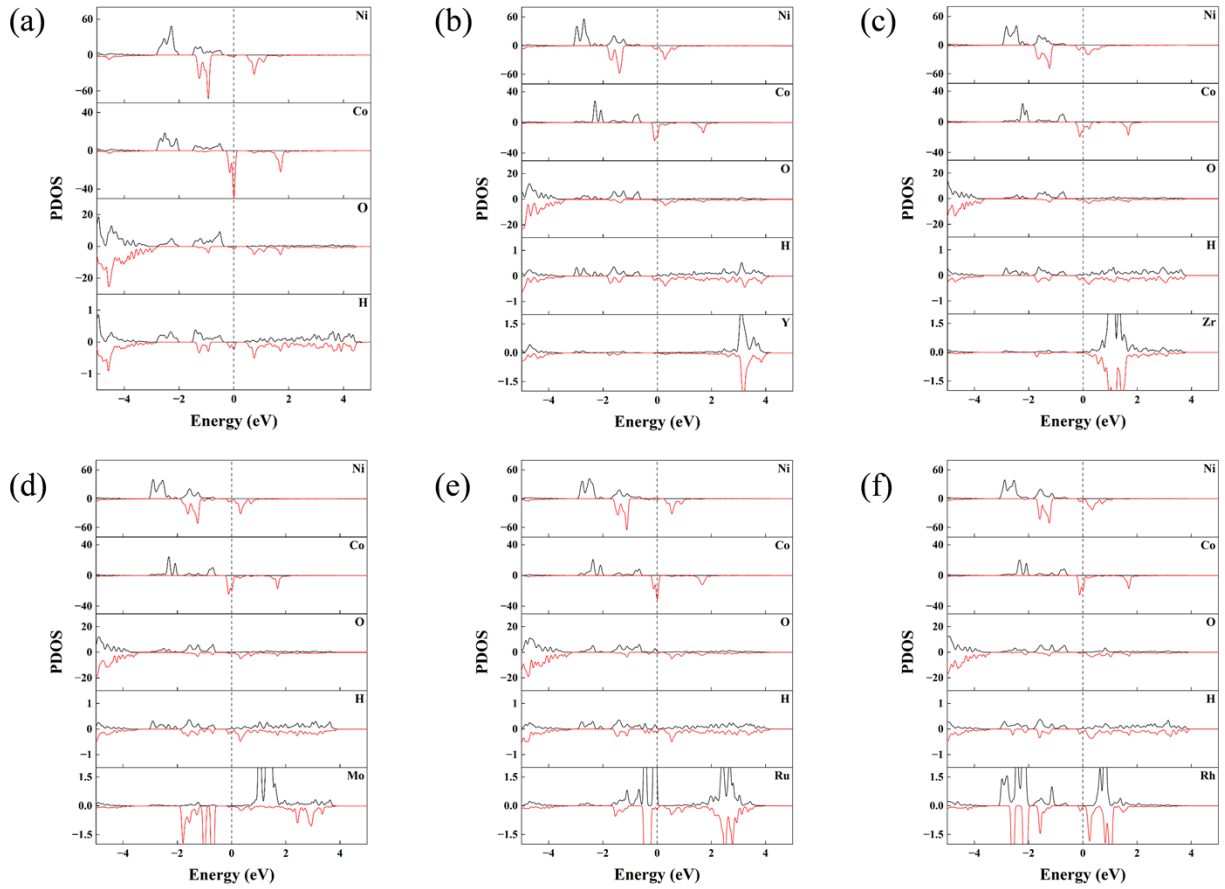

Figure S7. Projected density of states (PDOS) for (a) pristine NiCo LDHs, and (b–f) Y-, Zr-, Mo-, Ru-, and Rh-doped NiCo LDHs, respectively. The Fermi level is set to 0 eV.

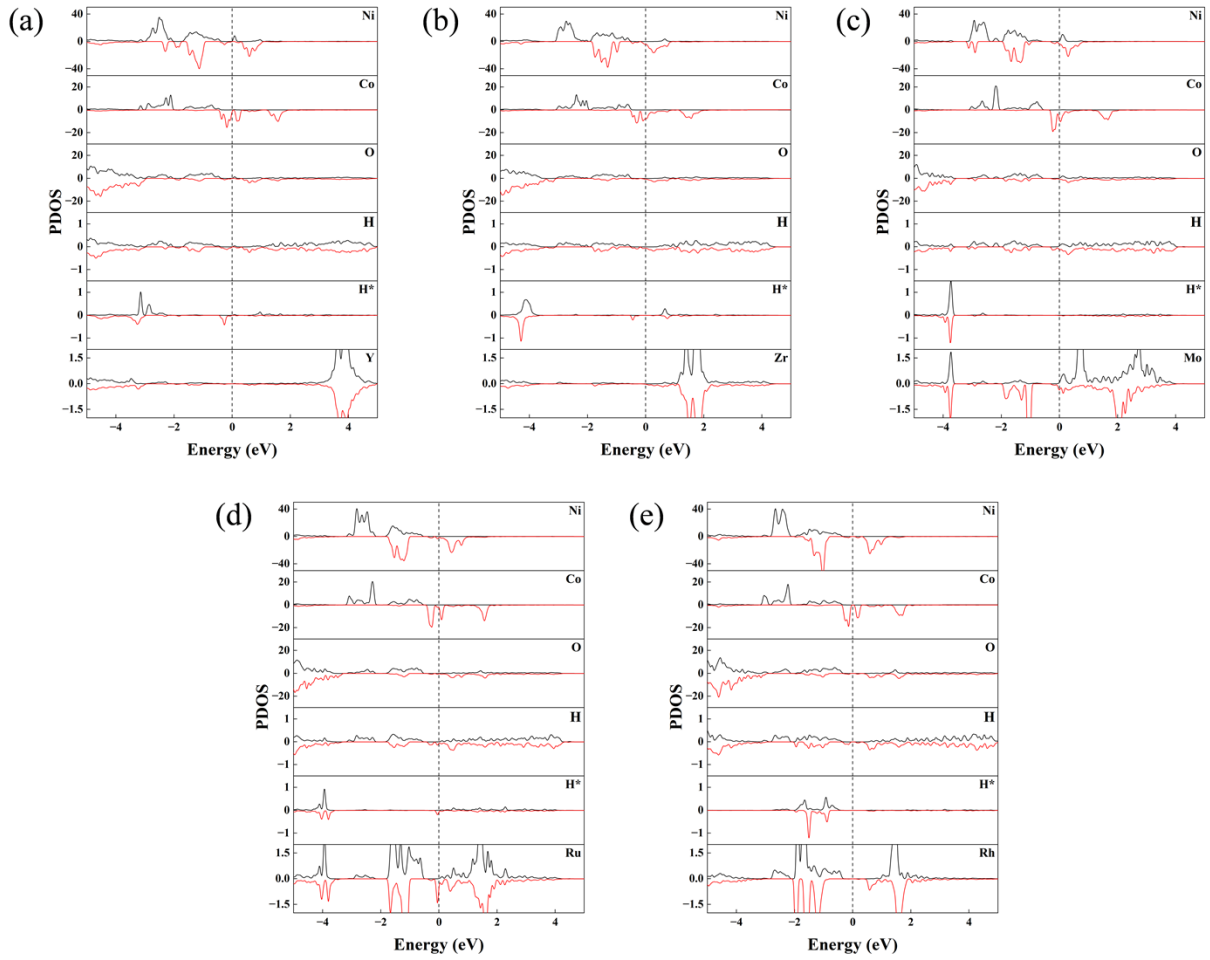

Figure S8. Calculated PDOS for the hydrogen adsorption configurations on NiCo LDHs doped with different 4d transition metals: (a) Y, (b) Zr, (c) Mo, (d) Ru, and (e) Rh. The Fermi level is aligned to 0 eV.

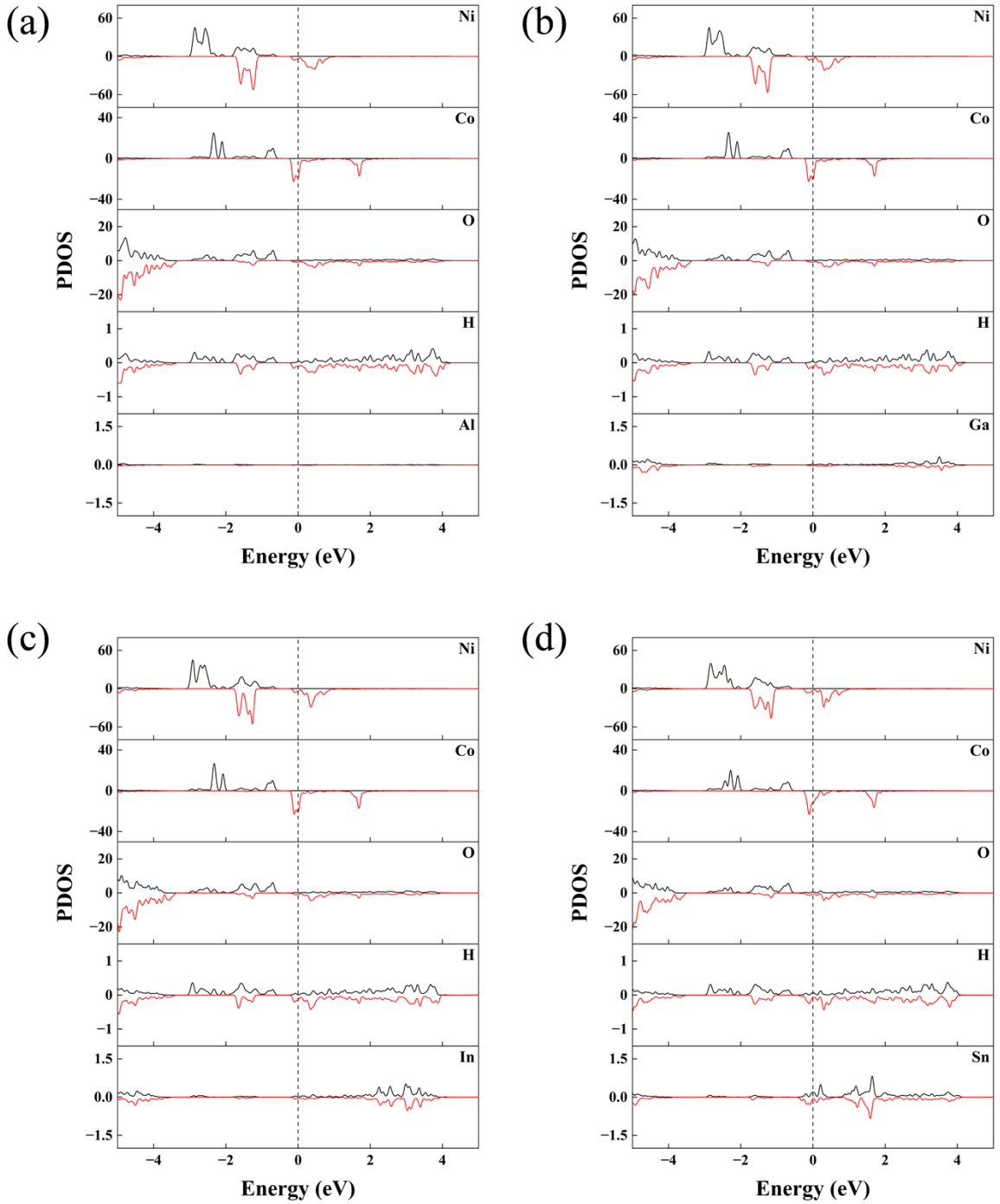

Figure S9. Projected density of states for Al-, Ga-, In-, and Sn-doped NiCo LDHs configurations.

The Fermi level is set to 0 eV.

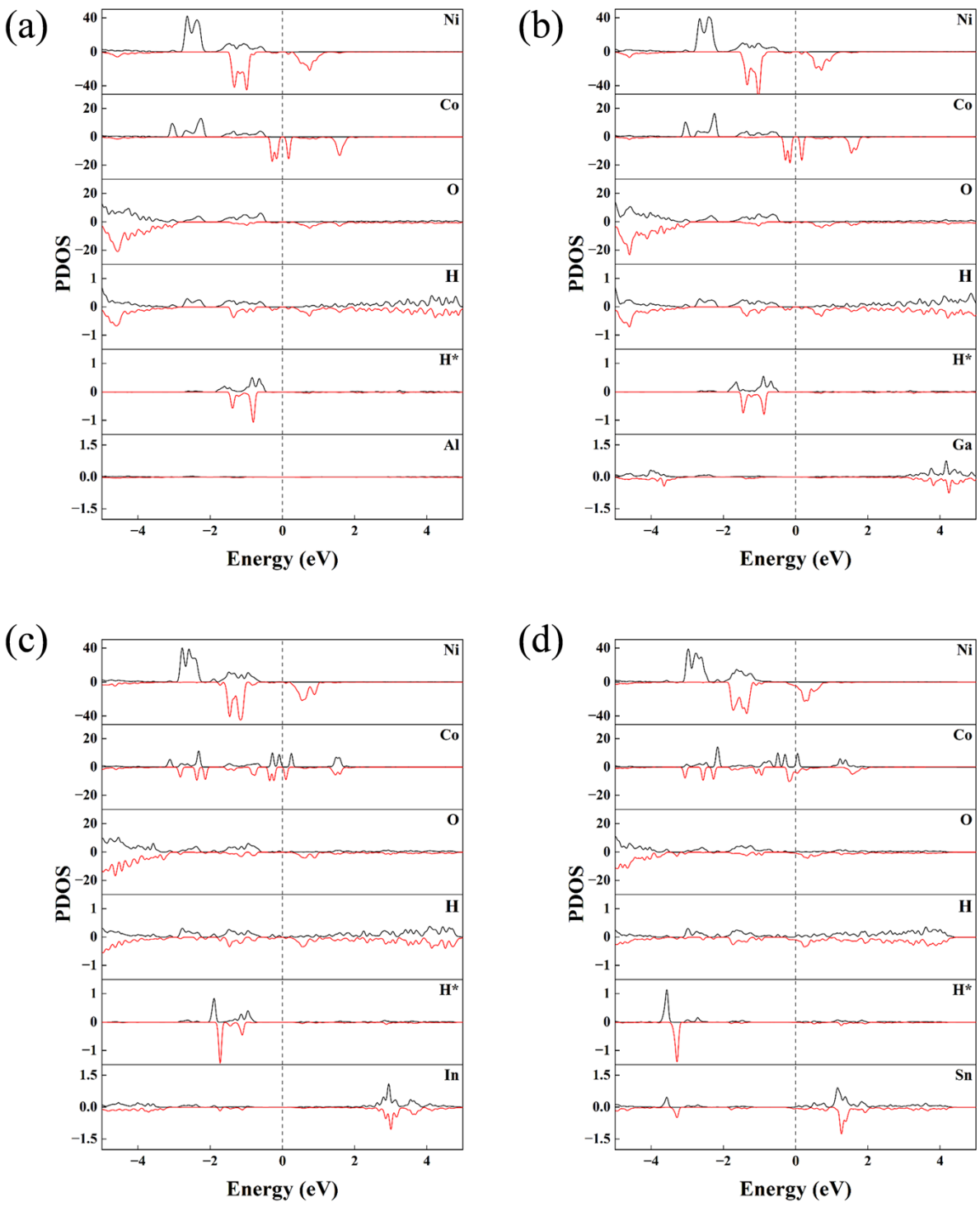

Figure S10. PDOS for the hydrogen adsorption configurations of (a–d) Al-, Ga-, In-, and Sn-doped NiCo LDHs, respectively. The Fermi level is set to 0 eV.