Supporting Information for "High-Performance Hydrogen Evolution Reaction Catalysts in three-dimensional single nodal loop semimetals ScX (X= Cd/Ag/Cu/Rh)"

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We calculated the band structure of ScCd doped with electrons, as shown in Fig S1, and it can be seen that after doping with electrons, their energy bands only move down without any other changes. The topological properties were not destroyed during the doping process, so its catalytic performance was not catastrophically affected.

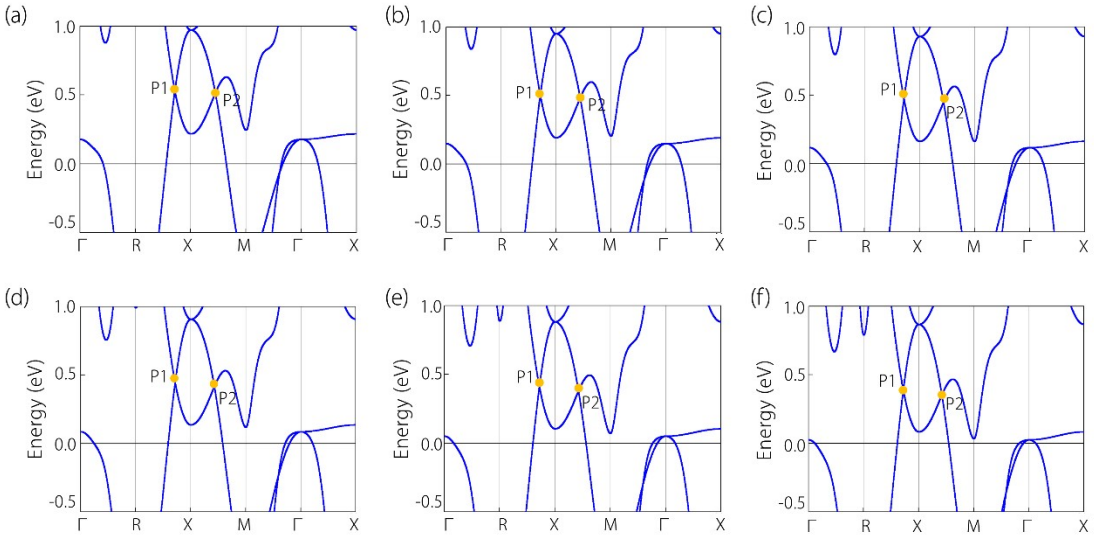

Figure S1. Energy band structure for ScCd with doping electrons (b-f). Here, the number of electrons from Figure (a) to Figure (f) is 0, 0.1, 0.2, 0.3,0.4 and 0.5.

The key step in studying the catalytic performance of materials is to determine the adsorption sites on the material surface. Taking the (001) surfaces as example, as shown in Fig S2 (a), it shows the atom arrangements on (001) surface, indicating three different

sites. These three sites are located directly above the Cd atom, directly above the Sc atom, and on the bridge sites of the two Sc (Cd) atoms, named as S1, S2, S3. By calculating the adsorption energy (ΔE_{ads}), we determined that the optimal adsorption site on the (001) surface is the S3 site, as shown in Fig S2 (b). In addition, we also performed similar calculations on four additional surfaces: (110), (111), (210), and (310), corresponding to Figures S3-S6 respectively.

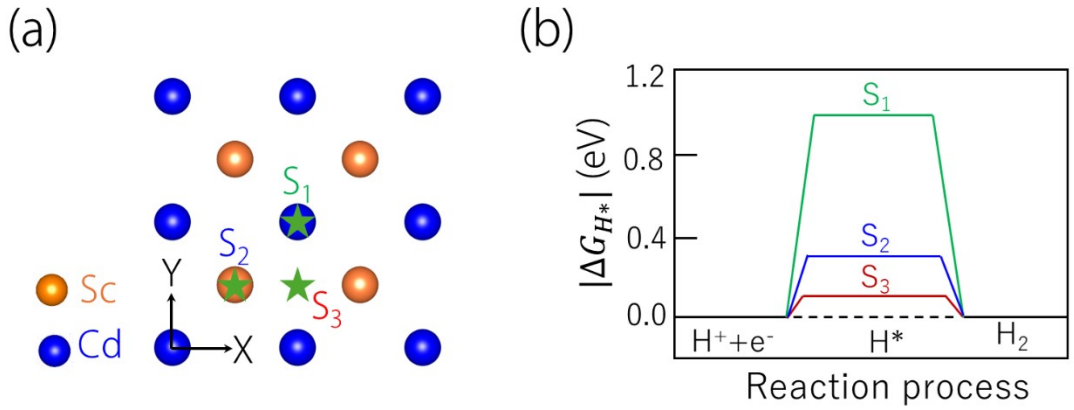

Figure S2. (a) Schematic diagram of adsorption sites on ScCd (001) surface. (b) Comparison graph of Gibbs free energy ($|\Delta G_{H^*}|$) between ScCd (001) surface various sites.

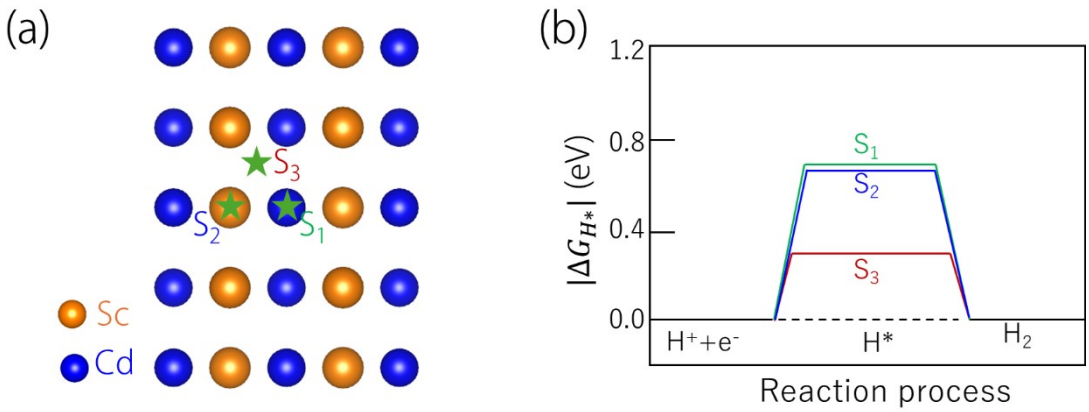

Figure S3. (a) Schematic diagram of adsorption sites on ScCd (110) surface. (b) Comparison graph of Gibbs free energy ($|\Delta G_{H^*}|$) between ScCd (110) surface various sites.

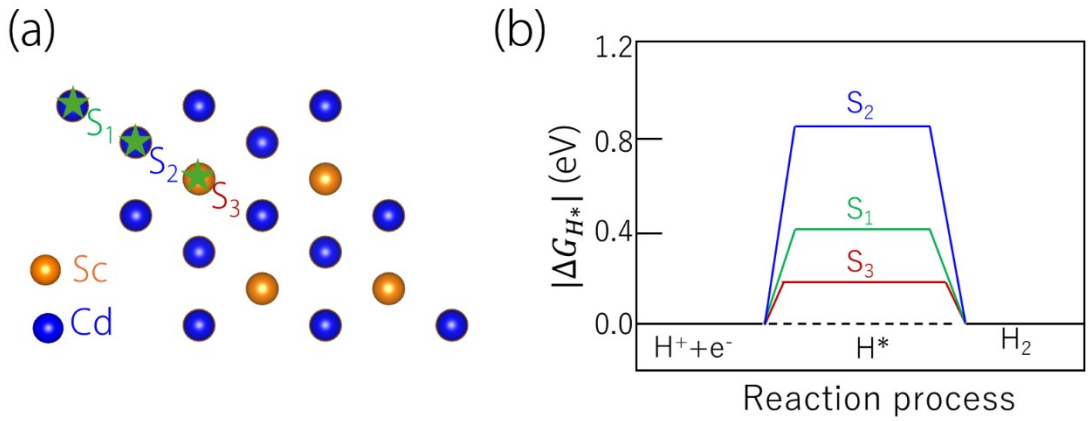

Figure S4. (a) Schematic diagram of adsorption sites on ScCd (111) surface. (b) Comparison graph of Gibbs free energy ($|\Delta G_{H^*}|$) between ScCd (111) surface various sites.

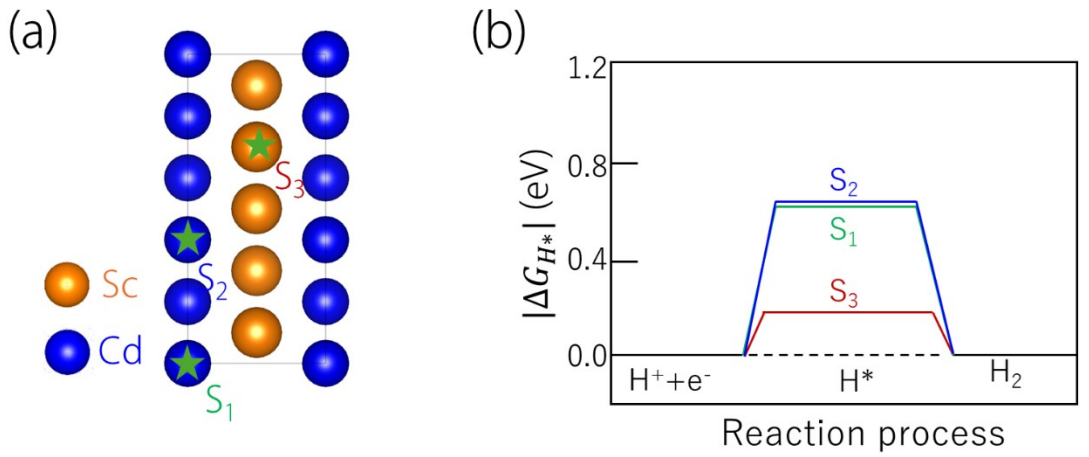

Figure S5. (a) Schematic diagram of adsorption sites on ScCd (210) surface. (b) Comparison graph of Gibbs free energy ($|\Delta G_{H^*}|$) between ScCd (210) surface various sites.

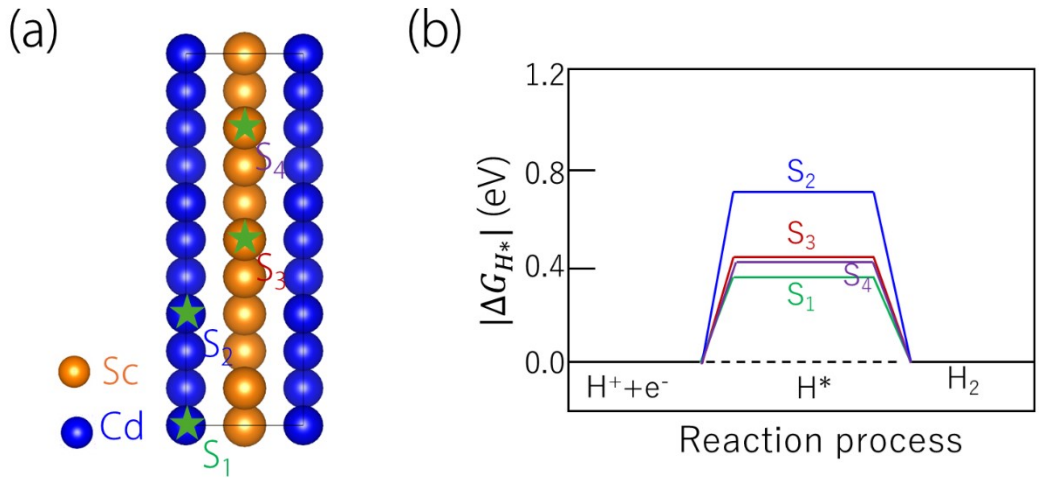

Figure S6. (a) Schematic diagram of adsorption sites on ScCd (310) surface. (b) Comparison graph of Gibbs free energy ($|\Delta G_{H^*}|$) between ScCd (310) surface various sites.

To enhance the accuracy of our calculation results, we employed implicit solvent correction and recalculated the Gibbs free energy (ΔG_{H^*}). As depicted in Fig S7(a), it is evident that the ΔG_{H^*} values on various ScCd surfaces exhibited minimal changes after the correction, with the ScCd (001) surface maintaining catalytic performance comparable to that of the precious metal Pt. Furthermore, as illustrated in Fig S7(b), it continues to adhere to the trend where ΔG_{H^*} varies linearly with the surface DOS.

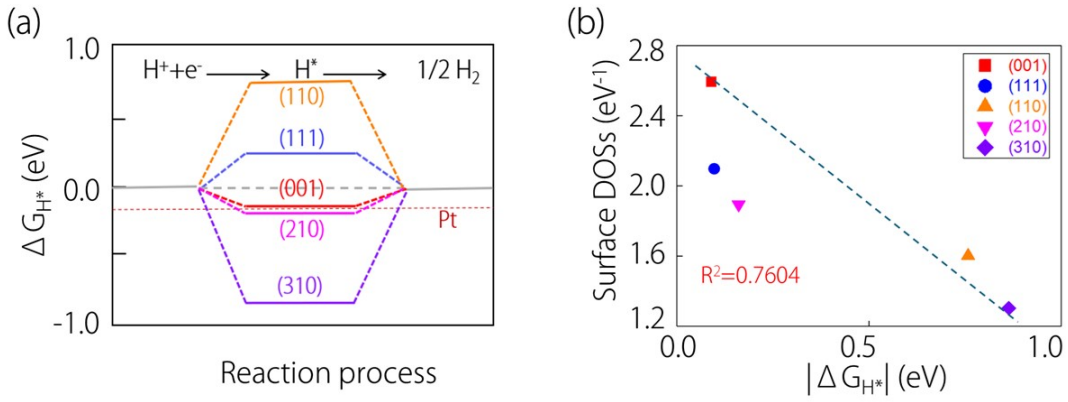

Figure S7. (a) Comparison graph of ΔGH* between ScCd various surfaces and metal Pt after implicit solvent correction. (b) The relationship between SDOS and ΔGH* of ScCd with different surfaces after implicit solvent correction.

We calculated the band structure after applying biaxial strain, specifically applying a biaxial strain ranging from 0% to 10% on the xy axis of the ScCd lattice, as illustrated in Figure S8. The results demonstrate that applying biaxial strain preserves lattice symmetry, maintains nodal loops unbroken, and consequently sustains catalytic performance at a level comparable to that of precious metal Pt.

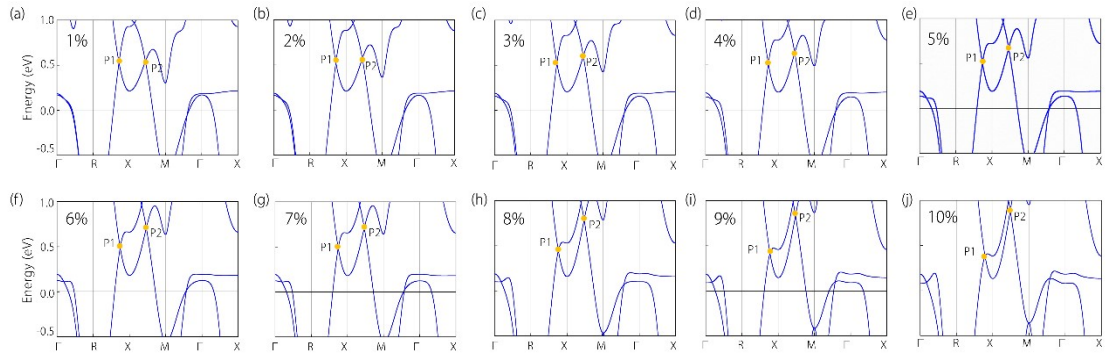

Figure S8. Energy band structure for ScCd with biaxial strain (a-j). Here, the number of biaxial strain from Figure (a) to Figure (j) is 0%-1%.

Other material candidates, namely ScRh, ScCu, and ScAg, that they have topological properties similar to ScCd. As shown in Fig S9, we present the band structures of these three materials. In addition, we also preliminarily predicted the potential of these three materials as HER catalysts. We calculated the ΔG_{H^*} of these three materials, as shown in Fig S9 (d). Their ΔG_{H^*} values are lower than those of traditional precious metal catalysts Pt. Indicating that they have excellent catalytic performance.

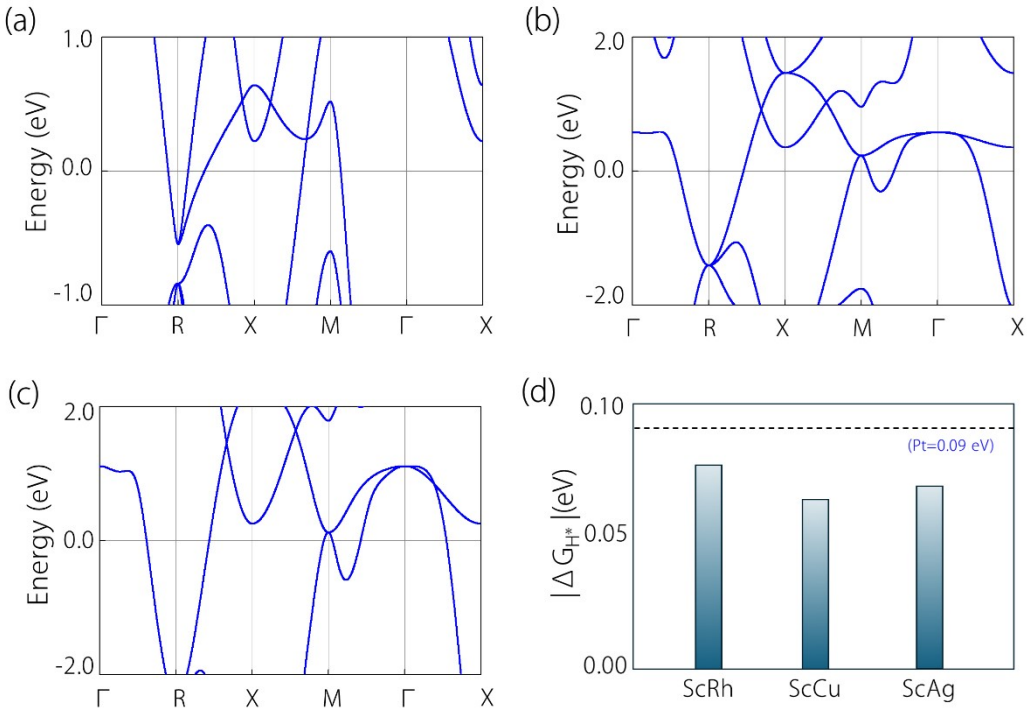

Figure S9. The energy band diagrams of three topological materials, namely ScRh

(a), ScCu (b), and ScAg (c). (d) Comparison graph of ΔG_{H^*} between ScRh, ScCu and ScAg.