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Electrocatalytic activity of β-Sb two-dimensional surface for hydrogen evolution reaction

Mengya Yang[1], Xiaoyan Ren[1], Shunfang Li[1], Yingjiu Zhang[2], Xinjian Li[2], Rui Pang[1*], Yuanyuan Shang[2*]

[1]International Laboratory for Quantum Functional Materials of Henan, School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450001, PR China

[2]Key Laboratory of Material Physics, Ministry of Education, School of Physics and Microelectronics, Zhengzhou University, Zhengzhou 450052, PR China

*Corresponding authors: pangrui@zzu.edu.cn, yuanyuanshang@zzu.edu.cn

Supporting Information:

Fig. S1 The optimized β-Sb structure diagram shows (a) side view; (b) top view. (c) The temperature fluctuation at 300 K of the Te@Sb structure as a function of the ab initio molecular dynamics (AIMD) simulation time. The time-step is 1 fs.

Fig. S2 (a) The ΔG_{H^*} and formation energies of the As@Sb structure at 5 and 15 valence electrons, and (b) the ΔG_{H^*} at 400eV, 450eV, and 500eV of the As@Sb structure.

Fig. S3 The lowest energy configurations of the adsorption behavior of H atom on the surface of (a) pristine β-Sb monolayer, (b) P@Sb, (c) As@Sb, (d) O@Sb, (e) S@Sb, (f) Se@Sb, and (g) Te@Sb structures.

Fig. S4 The relationship between spin-orbit coupling and HER catalysis.

Fig. S5 (a) The structure of doped atomic. (b) Formation energy increases with doping concentration.

Fig. S6 The Te@Sb structure applies biaxial compressive strain in the *x* and *y* directions.

Fig. S7 The relationship between the number of electrons transferred from activated Sb atoms to Se and As dopants and the ability of Se@Sb structure and As@Sb structure to trap hydrogen atoms, respectively.

Fig.S8 Atom-partial density of states (PDOS) of (a) β-, (b) As@, (c) O@, (d) S@, (e) Se@ and (f) Te@Sb.

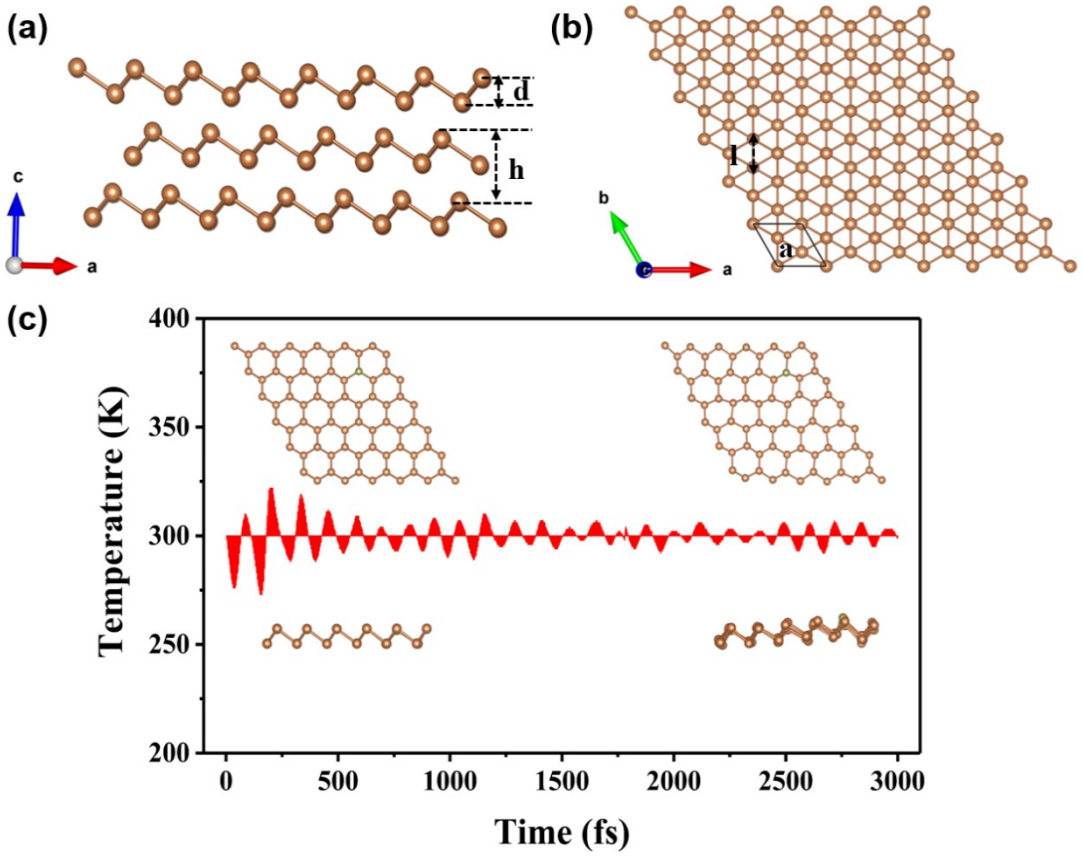
Fig. S9 The charge density difference profile with top and side views for H atom adsorbed on the surface of (a) P@Sb, (b) As@Sb, (c) O@Sb, (d) S@Sb, (e) Se@Sb, and (f) Te@Sb structures. Yellow/blue color represents the electron accumulation/depletion. The isovalue is set to 0.001 e/Å^3.

Fig. S10 The values of D@Sb-H structure under different vdW corrections (D=O, S, Se, Te).

Detailed data:

(1) Doping structure atomic coordinates (Cartesian).

(2) D@Sb-H structure atomic coordinates (Cartesian)



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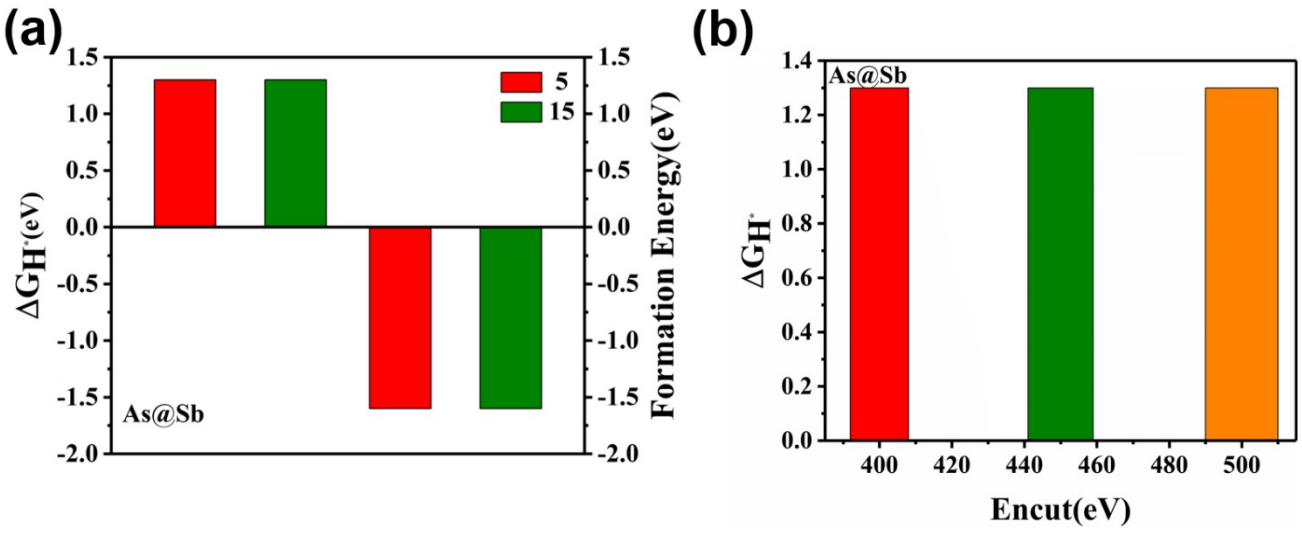


Fig. S2 (a) The $^{\Delta G_{H^*}}$ and formation energies of the As@Sb structure at 5 and 15 valence electrons, and (b) the $^{\Delta G_{H^*}}$ at 400eV, 450eV, and 500eV of the As@Sb structure.

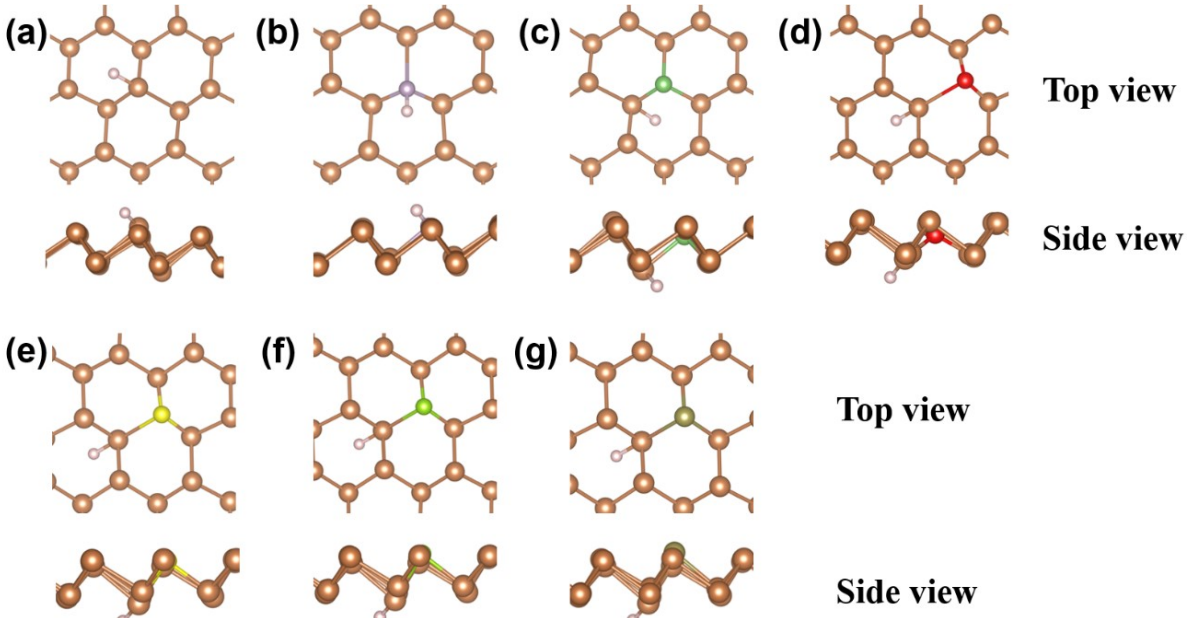


Fig. S3 The lowest energy configurations of the adsorption behavior of H atom on the surface of (a) pure β-Sb monolayer, (b) P@Sb, (c) As@Sb, (d) O@Sb, (e) S@Sb, (f) Se@Sb, and (g) Te@Sb structures.

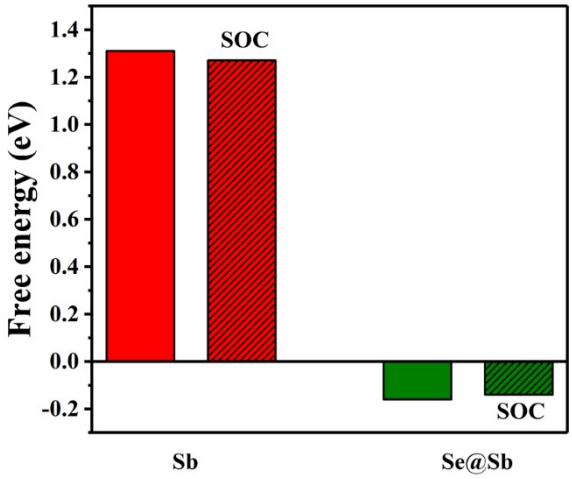
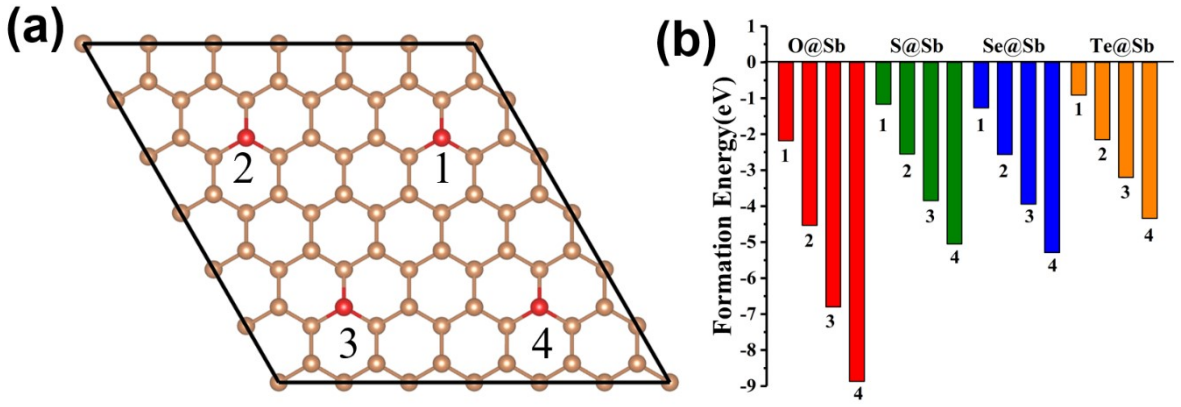


Fig. S4 The relationship between spin-orbit coupling and HER catalysis.



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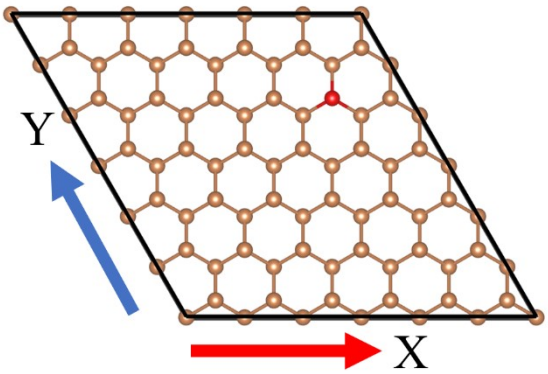

Fig. S6 The Te@Sb structure applies biaxial compressive strain in the x and y directions.

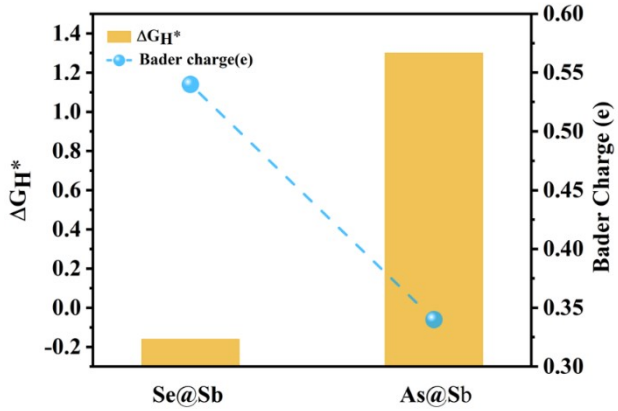

Fig. S7 The relationship between the number of electrons transferred from activated Sb atoms to Se and As dopants and the ability of Se@Sb structure and As@Sb structure to trap hydrogen atoms, respectively.

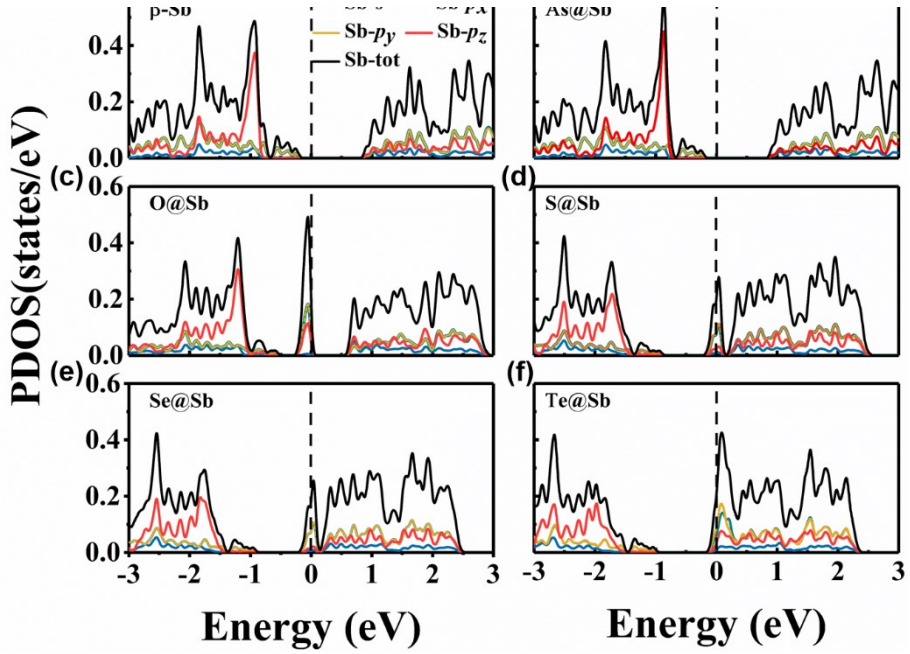

Fig.S8 Atom-partial density of states (PDOS) of (a) β-, (b) As@, (c) O@, (d) S@, (e) Se@ and (f) Te@Sb.

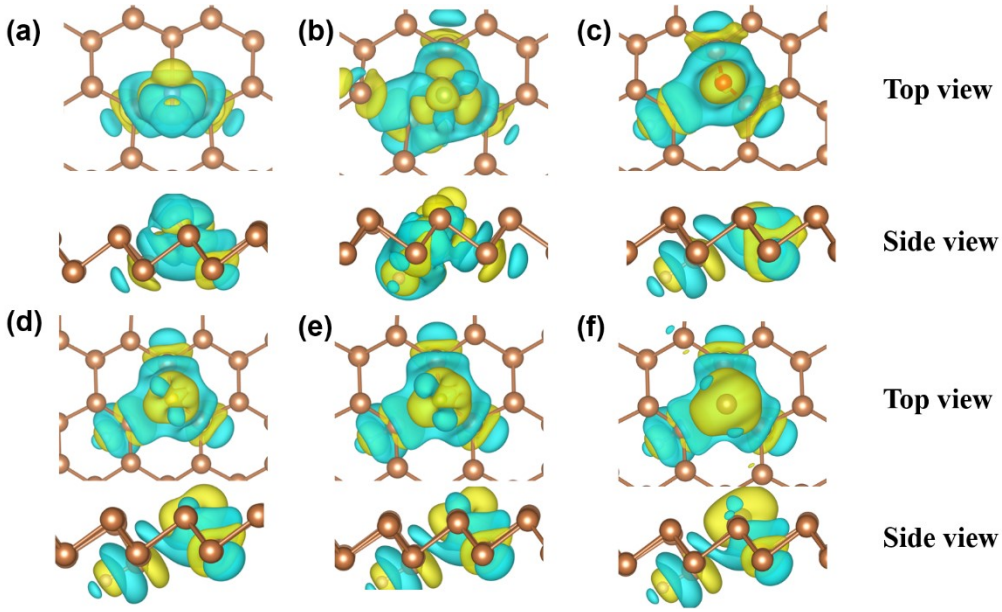

Fig. S9 The charge density difference profile with top and side views for H atom adsorbed on the surface of (a) P@Sb, (b) As@Sb, (c) O@Sb, (d) S@Sb, (e) Se@Sb, and (f) Te@Sb structures. Yellow/blue color represents the electron accumulation/depletion. The isovalue is set to 0.001 e/Å^3.

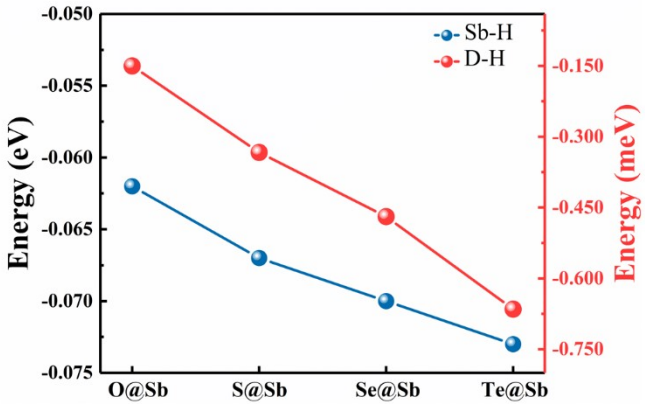

Fig. S10 The values of D@Sb-H structure under different vdW corrections (D=O, S, Se, Te).

Detailed data

(1) Doped structure atomic coordinates (Cartesian)

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Sb O
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