Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Single s-block and p-block metal sites for photocatalytic degradation of organic pollutants and hydrogen evolution

Yafei Zhao[a,*], Qiuze Li[a], Song Lu[d], Kuiying Nie[c], Xinzhong Li[a] and Liang He[b,*]

[a]*School of Physics and Engineering, Henan University of Science and Technology, Luoyang 471023, China*

[b]*National Laboratory of Solid State Microstructures, School of Electronic Science and Engineering and Collaborative Innovation Center of Advanced Microstructures, Nanjing University, Nanjing 210093, China*

[a]*College of Physics & Engineering Technology, Xingyi Normal University for Nationalities, Xingyi 562400, China*

[d]*Department of Energy and Petroleum Engineering, University of Stavanger, Stavanger 4036, Norway*

* Corresponding authors. *E*-mail: hzjlzhao@sina.com; heliang@nju.edu.cn

Supporting information

The structure, electronic, optical and photocatalytic properties of metal doped monolayer GeSe have been systematically studied by first principles calculations. It is noted that Se-rich growth condition is beneficial to the formation of metal doped GeSe. The band structure of IIA group (Be, Mg, Ca, Sr and Ba) and IVA group (Sn and Pb) doped GeSe is similar to undoped GeSe. The semiconducting behaviors of GeSe are modified by p-type [IA group (Li, Na, K, Rb and Cs)] or n-type [VA group (Sb and Bi)] doping. And, IIIA group (Al, Ga and In) and VA group (Sb and Bi) doping can induce ILs within the band gap of GeSe.

S1. The electronic properties of metal doped monolayer GeSe

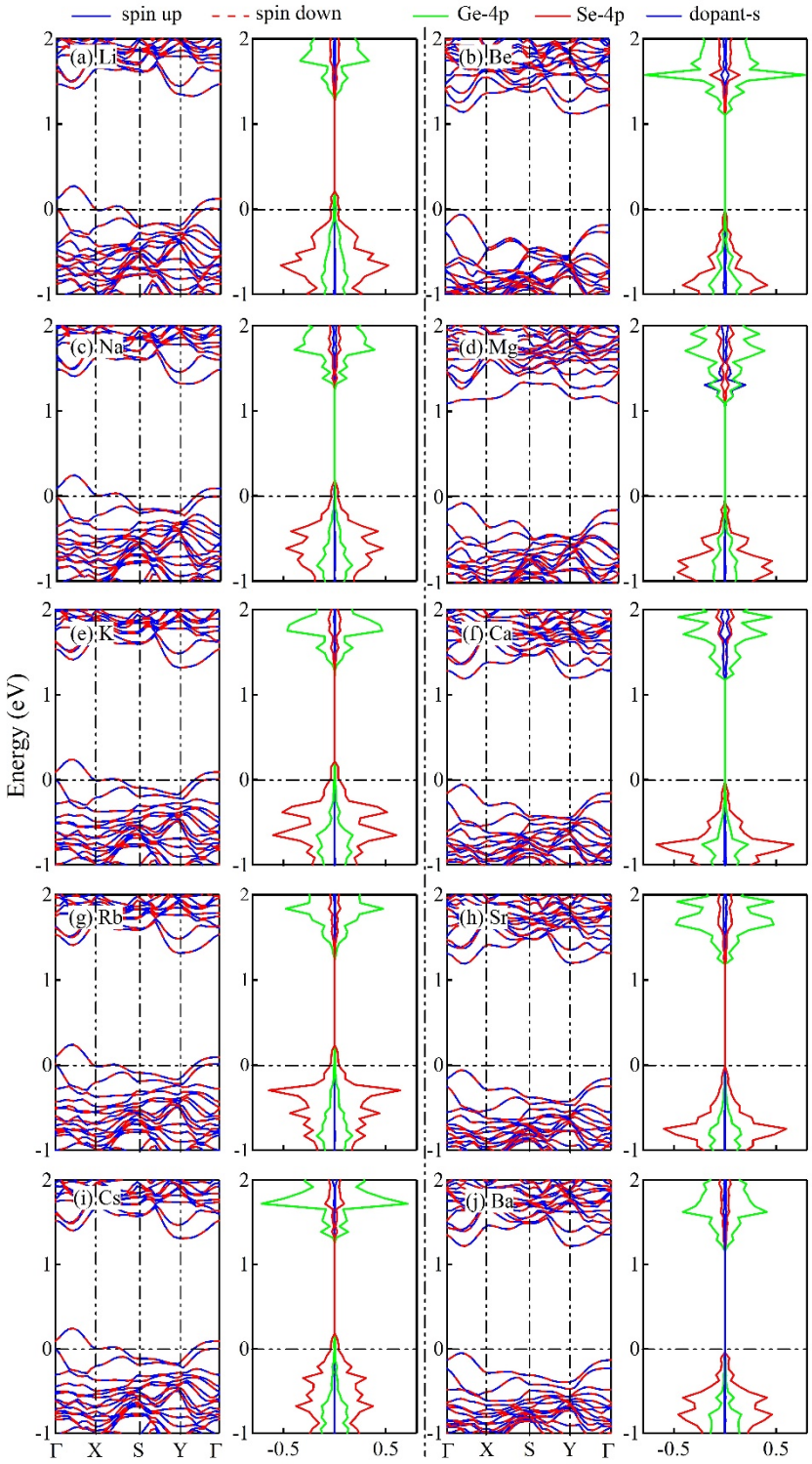

Figure S1. The band structure and average PDOS of IA and IIA group doped GeSe.

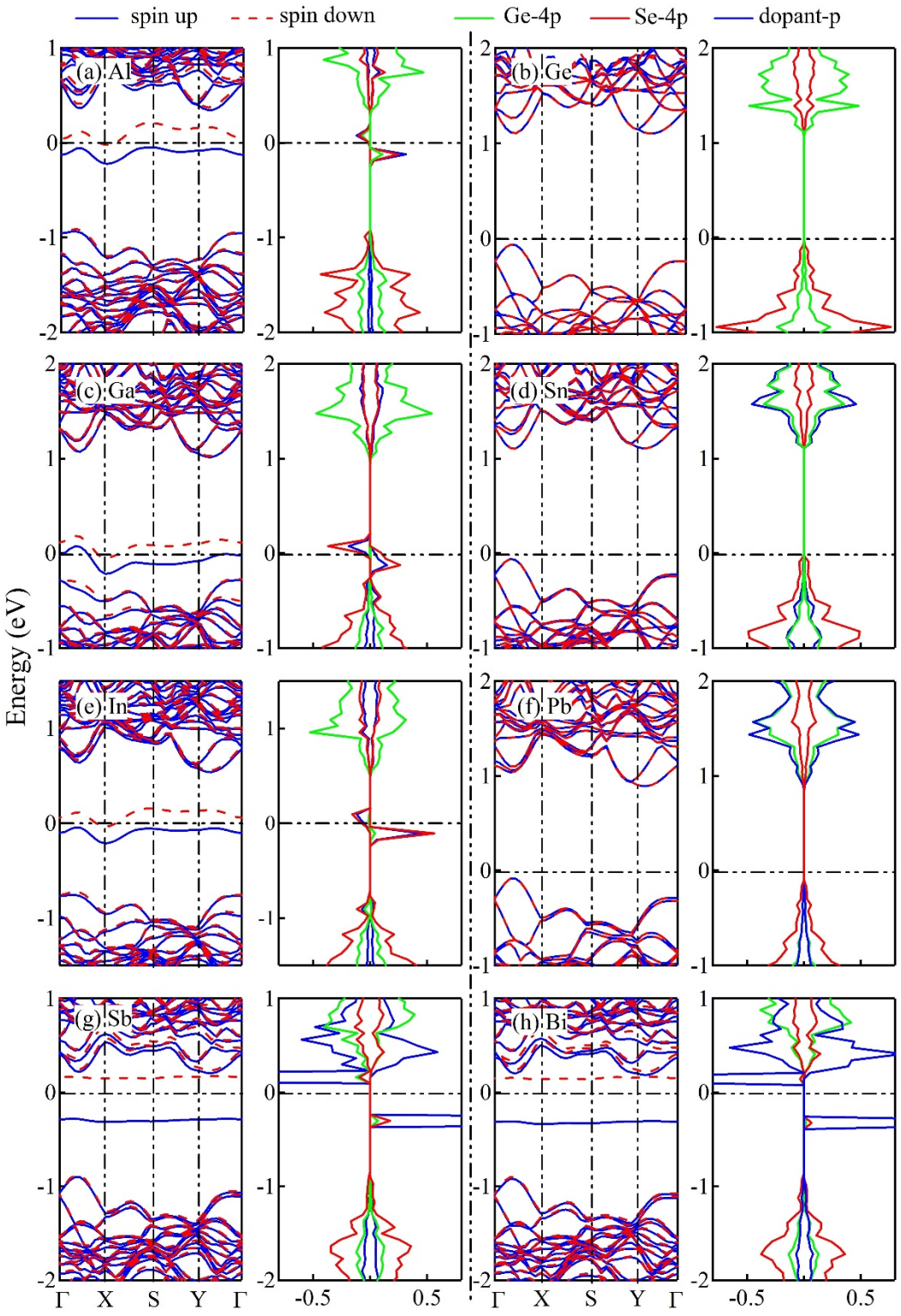

Figure S2. The band structure and average PDOS of IIIA, IVA and VA group metal doped GeSe.

S4. HOMO and LOMO states

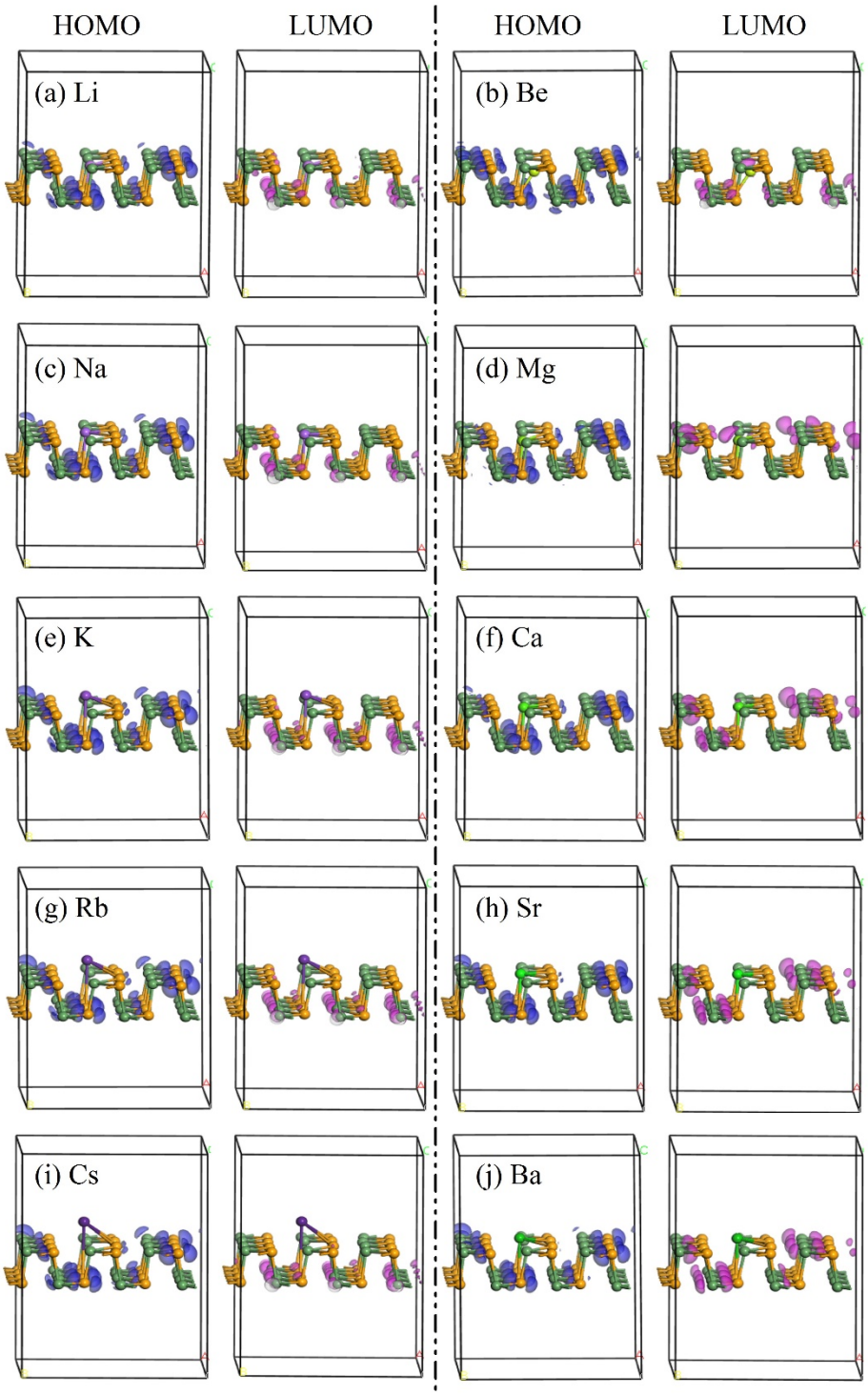

Figure S3. HOMO and LUMO of IA and IIA group metal doped monolayer GeSe. The separation of HOMO and LUMO contributes to the separation of photogenerated e^-/h^+.

Figure S4. HOMO and LUMO of IIIA, IVA and VA group metal doped monolayer GeSe.

S3. Optical absorption spectrum

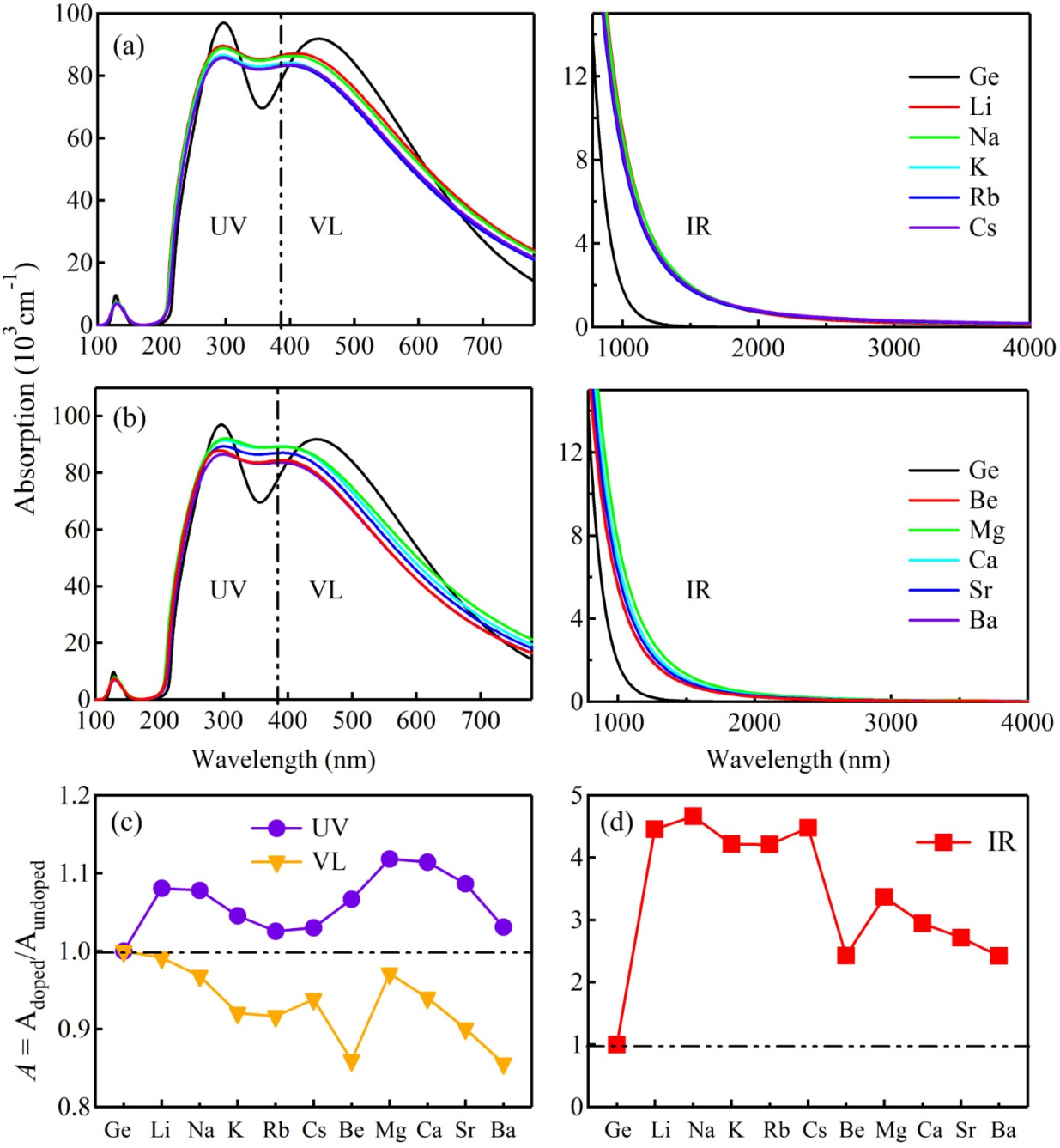

Figure S5. The optical absorption spectra of IA and IIA group metal doped GeSe.

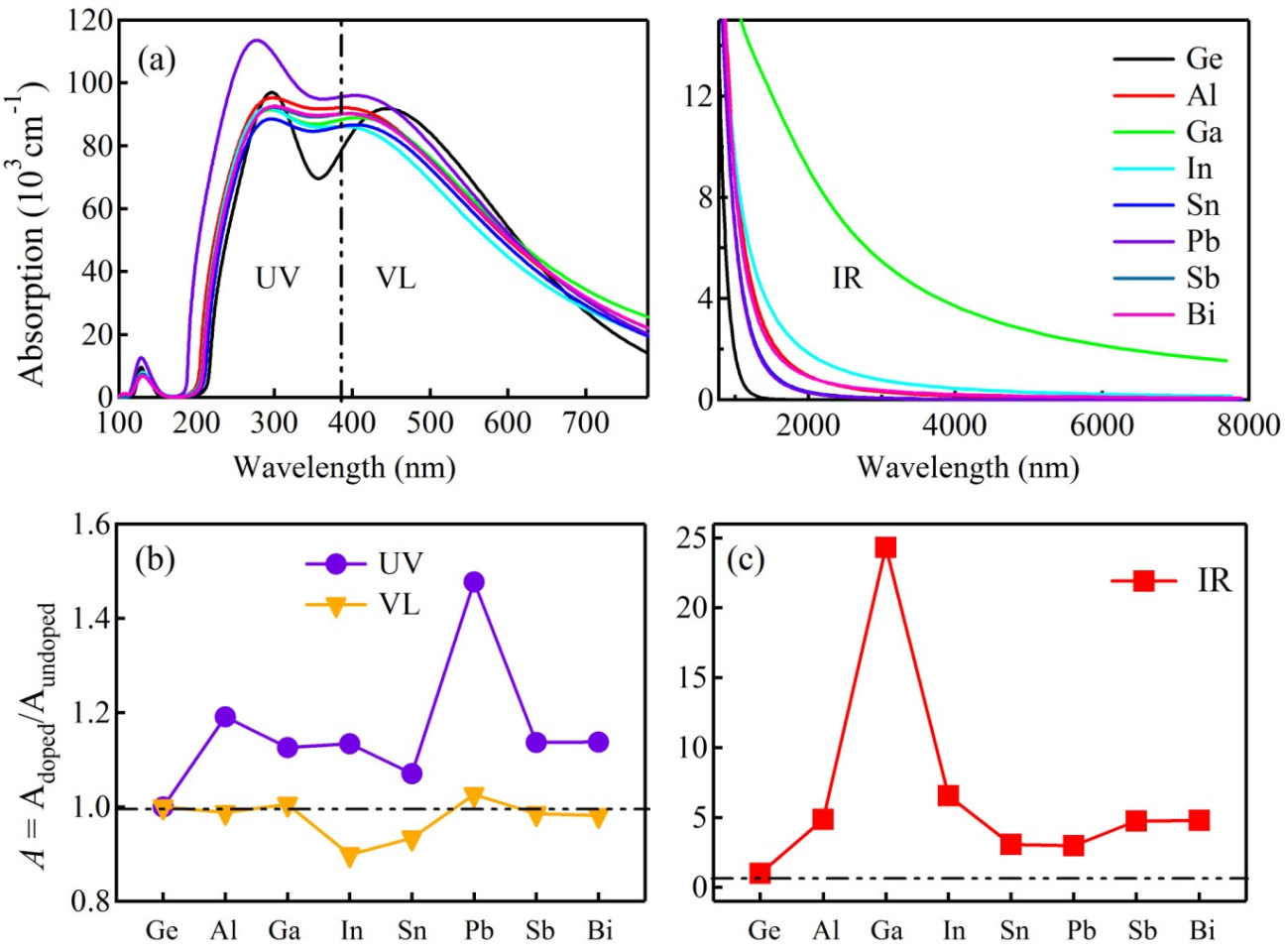

Figure S6. The optical absorption spectra of IIIA, IVA and VA group metal doped GeSe.

S4.Gibbs free energy diagram for H* adsorption (ΔG_H) on the different metal doped GeSe.

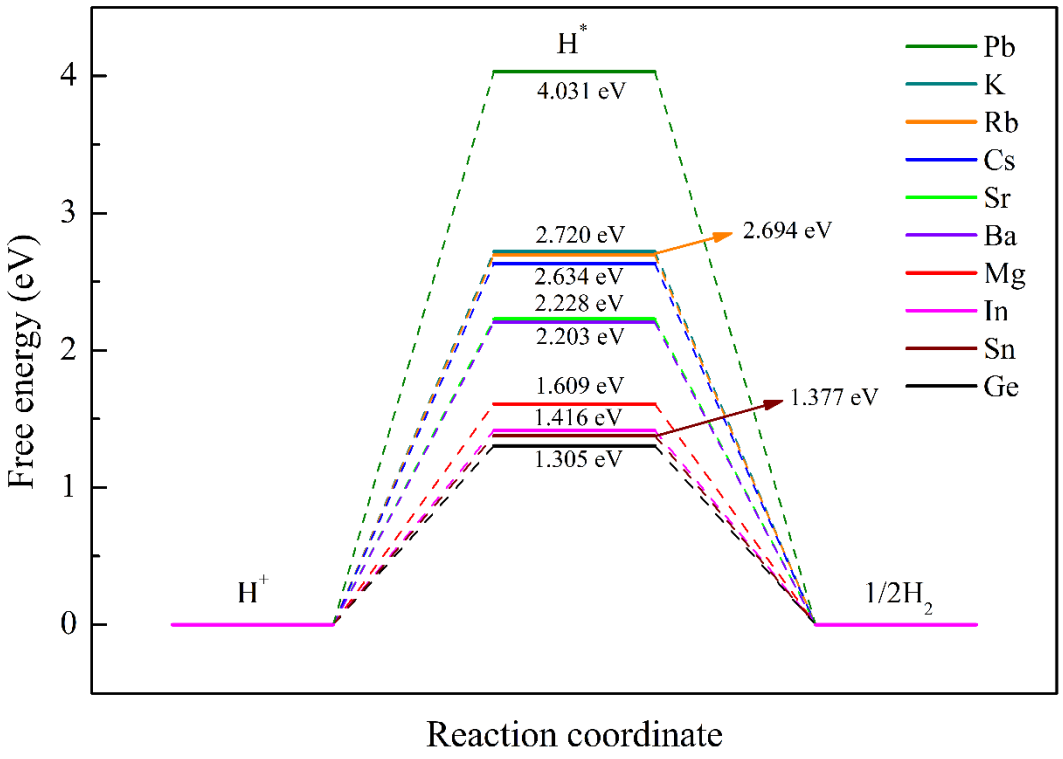

Figure S7. The ΔG_H of undoped and metal doped GeSe

S5. The energy position of band edge of the undoped and metal doped GeSe

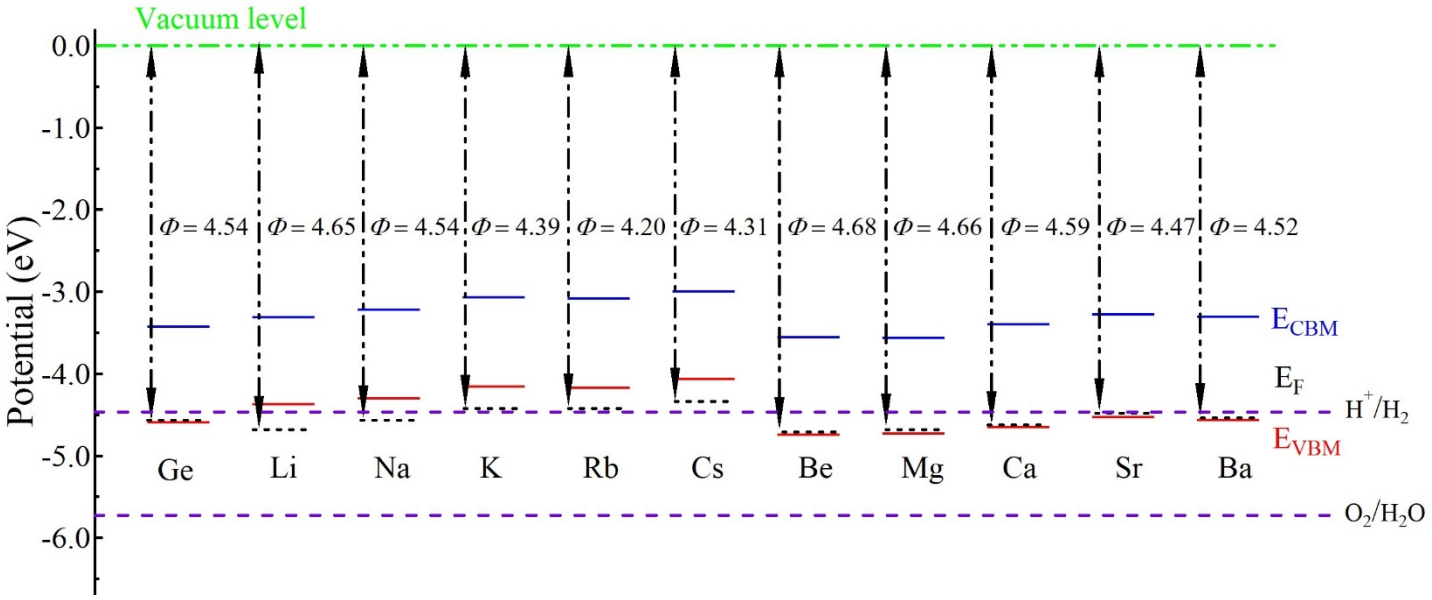

Figure S8. The energy of band edge and work function (Φ) of IA and IIA group metal doped system.

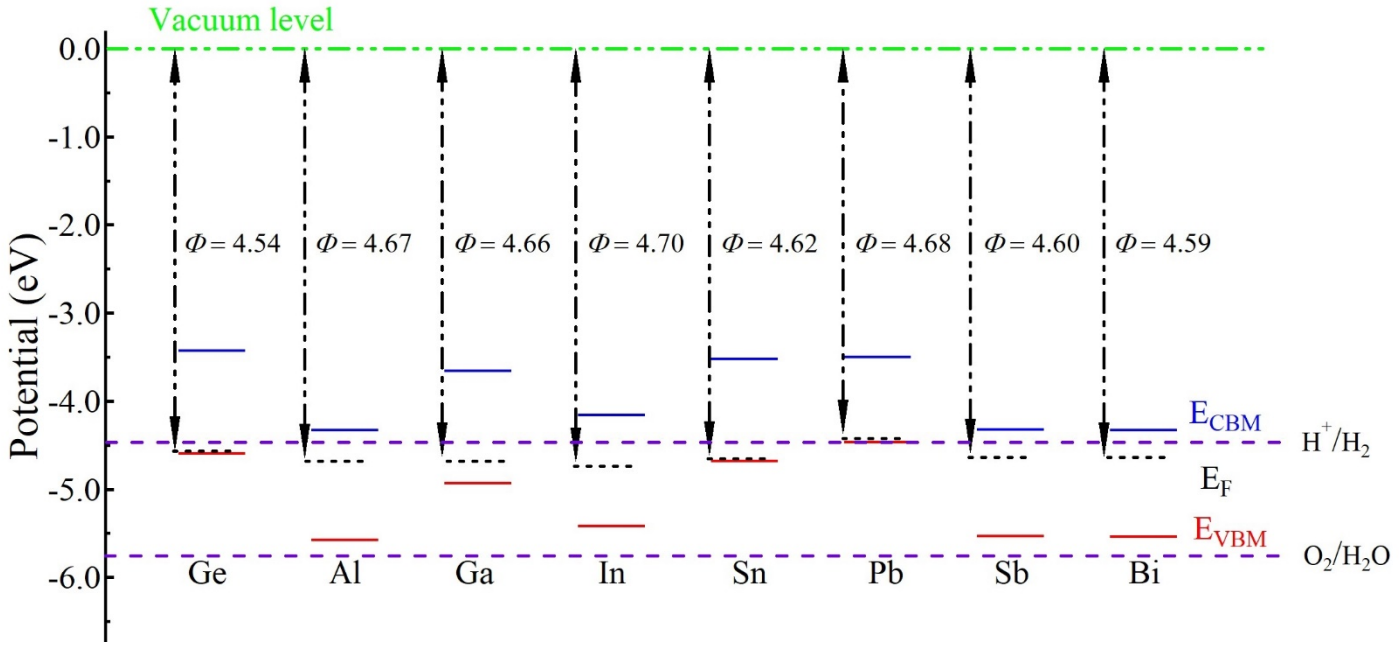

Figure S9. The energy of band edge and work function (Φ) of IIIA, IVA and VA group metal doped GeSe.

Table S1. The *a* and *b* are the lattice parameters, with unit Å. Δq is the charge transfer from doped metal atom to GeSe, *N* is the number of catalytic active sites.

Dopant	Na	K	Rb	Cs	Mg	Ca	Sr	Ba	Ga	In	Sn	Pb
a	4.267	4.299	4.301	4.287	4.245	4.267	4.293	4.331	4.267	4.350	4.307	4.360
b	3.944	3.950	3.950	3.947	3.976	3.995	3.999	3.997	3.961	3.937	3.986	3.886
Δq	0.87	0.91	0.90	0.92	1.43	1.37	1.52	1.70	0.63	0.89	0.74	0.88
N	23	24	24	25	23	23	25	25	22	17	25	23