

Coupling Co₂P/CoSe₂ heterostructure nanoarrays for boosting overall water splitting

Xiaoqiang Du^{a*}, Jiaxin Li^a, Kaicheng Tong^a and Xiaoshuang Zhang^b

^aSchool of Chemical Engineering and Technology, North University of China, Xueyuan road 3, Taiyuan 030051, People's Republic of China. E-mail: duxq16@nuc.edu.cn

^bSchool of Science, North University of China, Xueyuan road 3, Taiyuan 030051, People's Republic of China.

DFT calculation

In this study, the Cambridge Serial Total Energy Package module of Materials Studio was used for DFT calculation. The interactions of electrons were calculated by the generalized gradient approximation functions of Perdew-Burke-Ernzerh (GGA-PBE). The (111) plane optimal structures of Co₂P and CoSe₂ were calculated by setting a cutoff energy of 480 eV and 5×5×1 k-points grid. The structures were also optimized for energy and force convergence choosing as 2.0×10⁻⁵ eV/atom and 0.05 eV/Å, respectively. The vacuum space was up to 0.002 Å to eliminate periodic interactions.

Table S1. The atomic percent of Co₂P/CoSe₂-250

Element	Atomic %
O	39.54
C	35.46
Co	7.37
P	7.49
Se	10.14
Total:	100.00

Table S2. The atomic percent of Co₂P/CoSe₂-300

Element	Atomic %
O	40.12
C	35.56
Co	4.65
P	12.66
Se	7.02
Total:	100.00

Table S3. The atomic percent of Co₂P/CoSe₂-350

Element	Atomic %
O	41.69
C	34.20
Co	6.09
P	6.45
Se	11.57
Total:	100.00

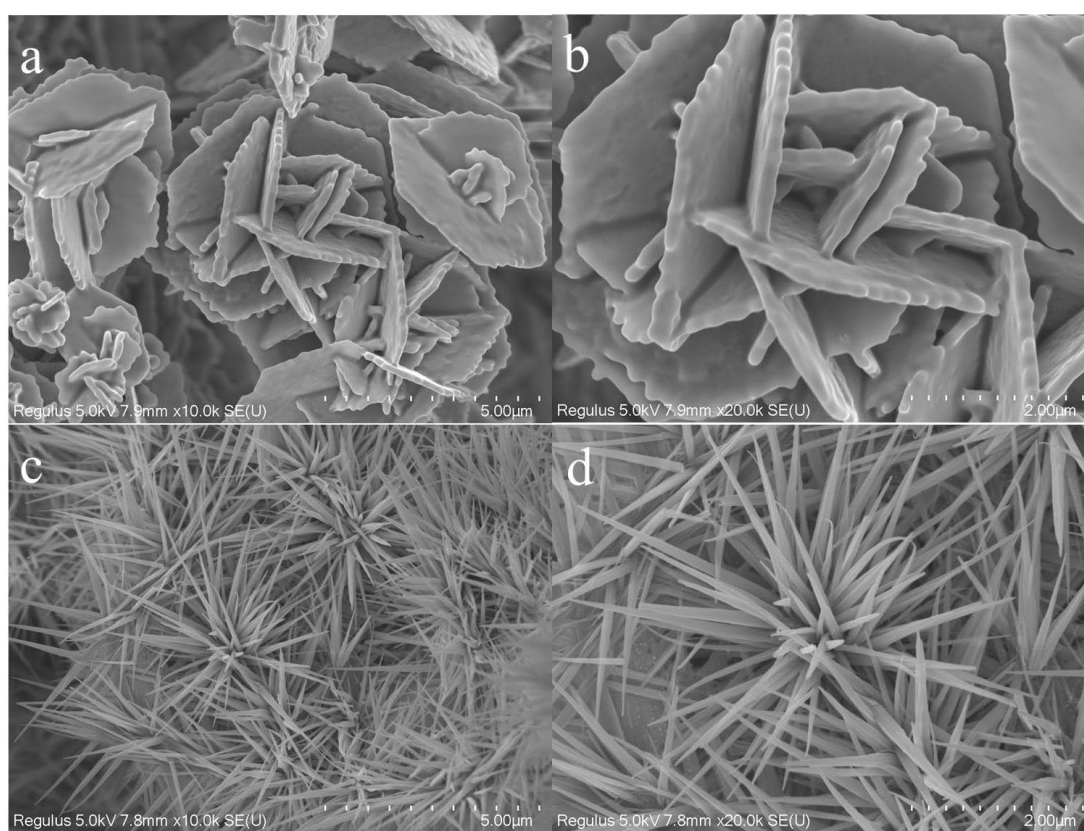


Fig. S1 SEM of the Co₂P/NF (a-b) and CoSe₂/NF (c-d).

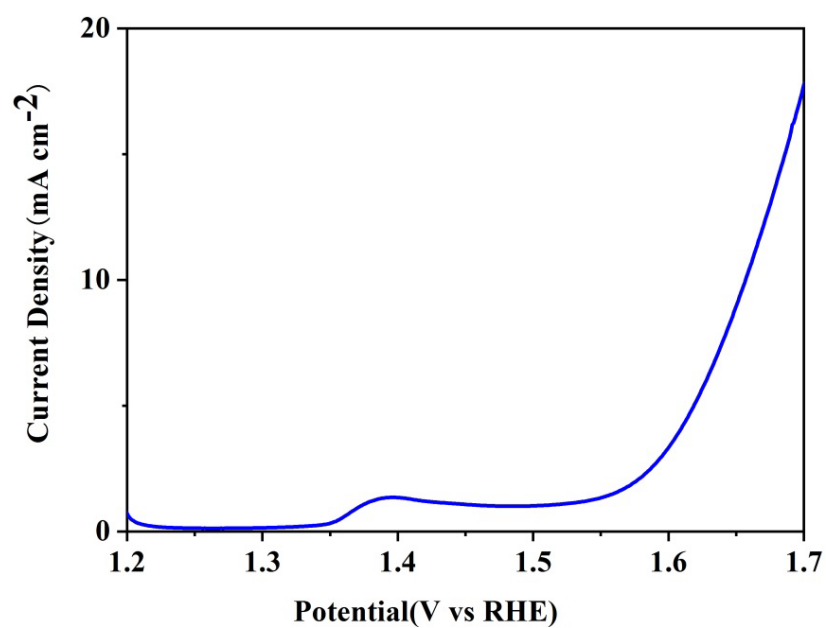


Fig. S2 Polarization curve of the Ni foam for OER with a scan rate of 5 mV s⁻¹ in 1 M KOH.

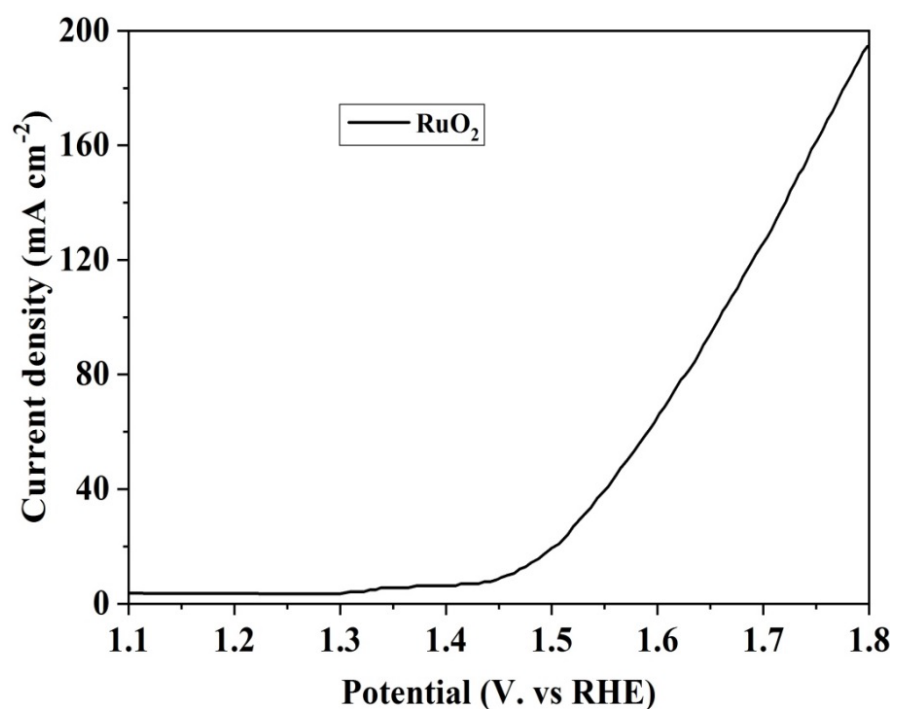


Fig. S3 Polarization curve of the RuO₂ for OER with a scan rate of 5 mV s⁻¹ in 1 M KOH.

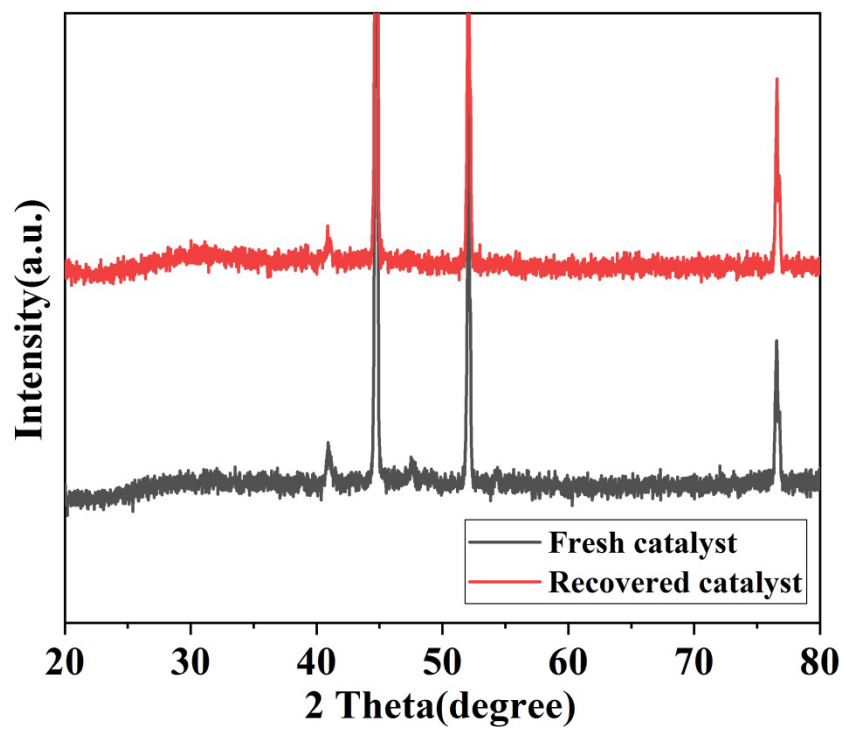


Fig. S4 XRD of the fresh and recovered $\text{Co}_2\text{P}/\text{CoSe}_2\text{-300}$.

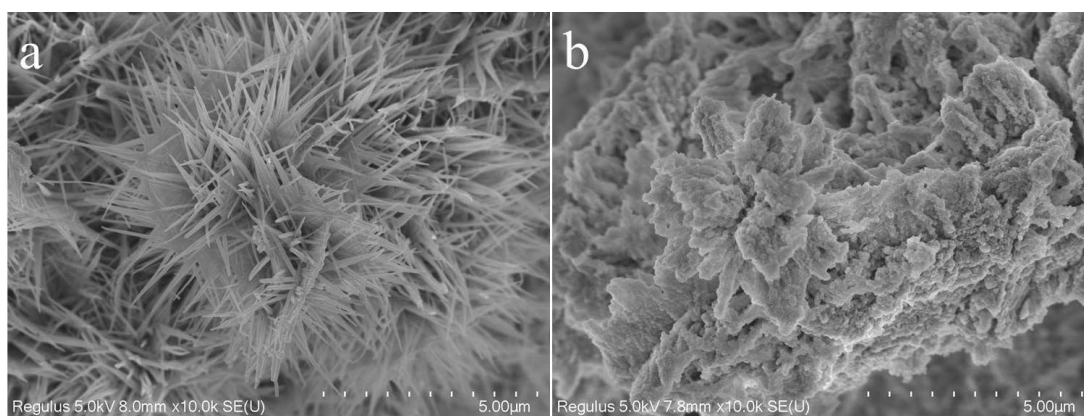


Fig. S5 SEM of the fresh and recovered $\text{Co}_2\text{P}/\text{CoSe}_2\text{-300}$.

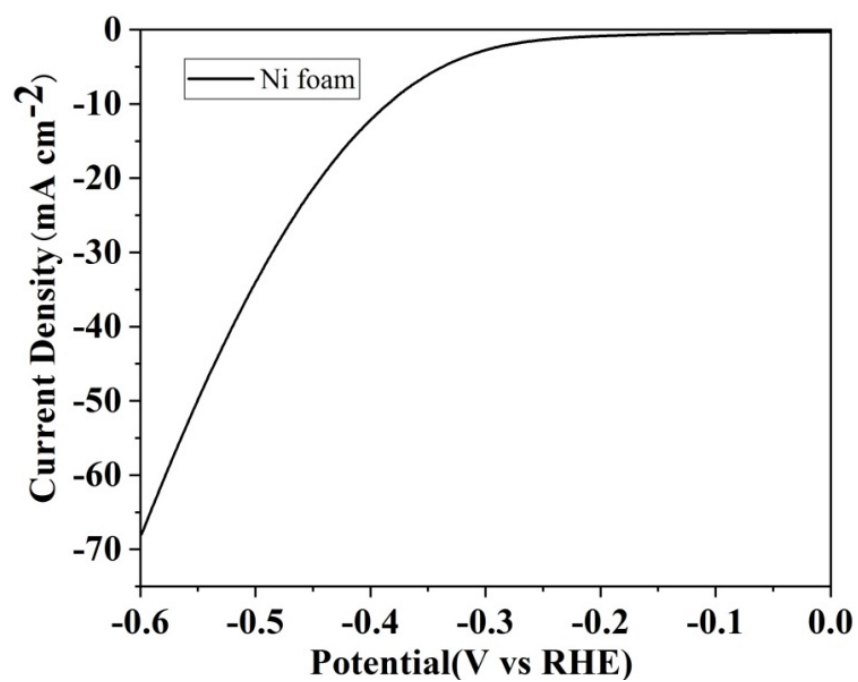


Fig. S6 Polarization curves of NF in 1.0 M KOH at a potential sweep rate of 5 mV s⁻¹.

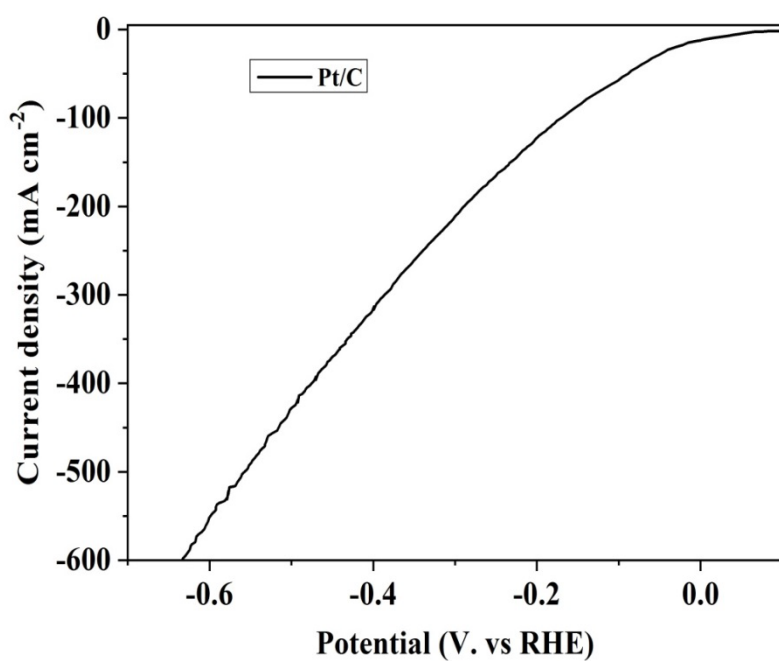


Fig. S7 Polarization curve of the Pt/C for HER with a scan rate of 5 mV s⁻¹ in 1 M KOH.

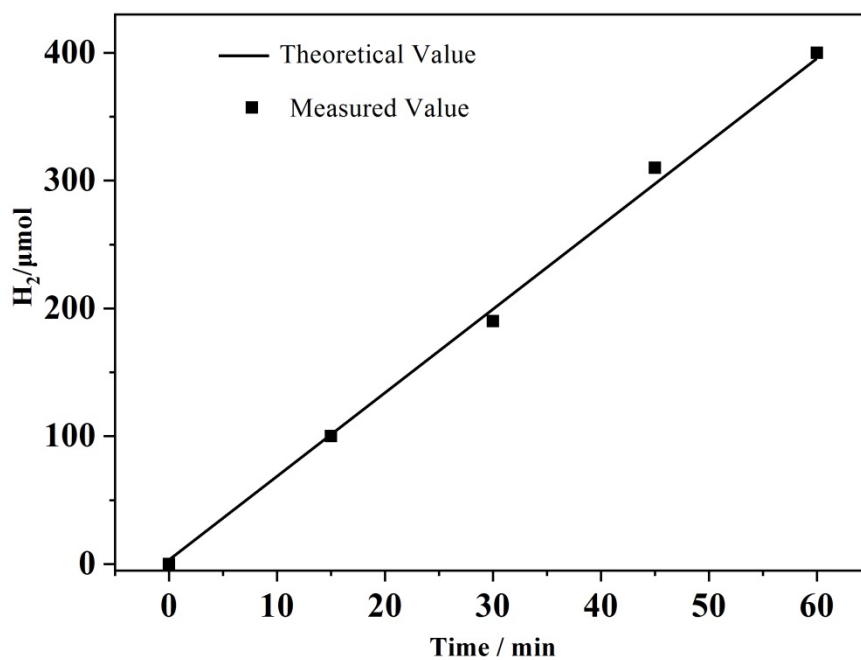


Fig. S8 Electrocatalytic efficiency of H₂ production over Co₂P/CoSe₂-300.

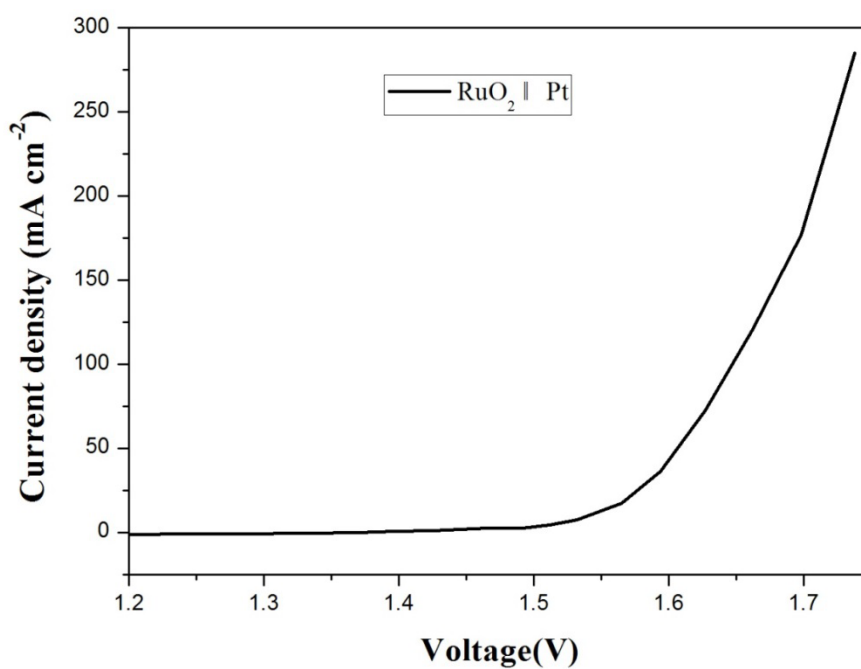


Fig. S9 Polarization curve of the RuO₂ and Pt for water splitting with a scan rate of 5 mV s⁻¹ in 1 M KOH.

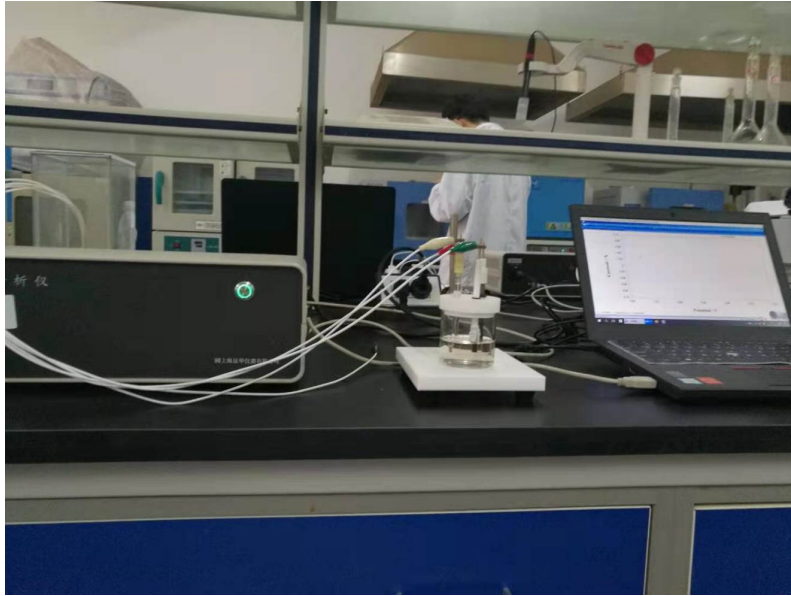


Fig. S10 Electrochemical testing equipment of the resulting materials.

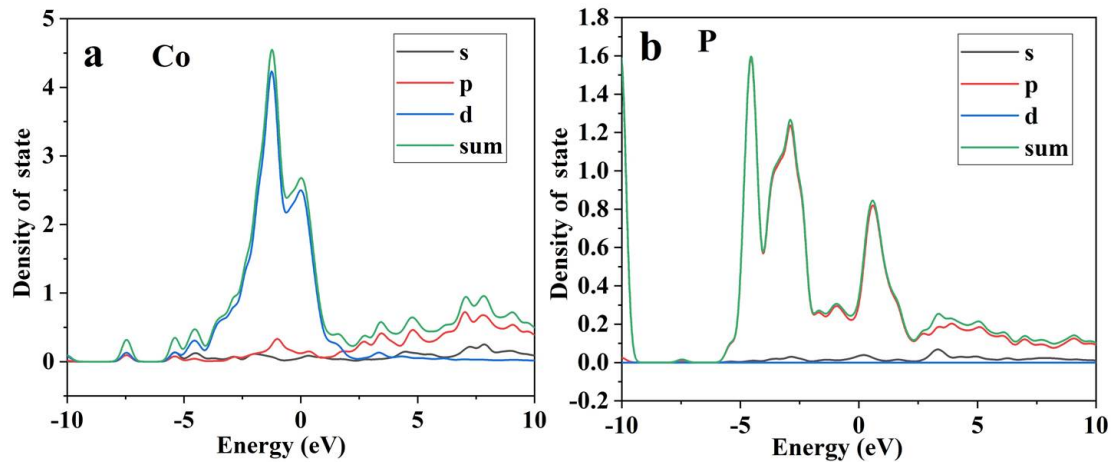


Fig. S11 Density of states for Co_2P , (a) Co and (b) P.

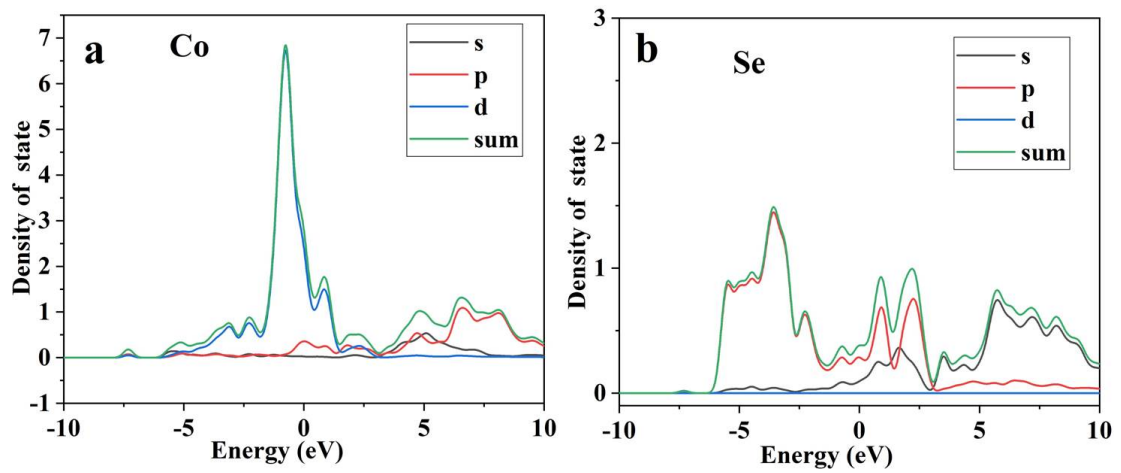


Fig. S12 Density of states for CoSe_2 , (a) Co and (b) Se.