

## Support Information

### Defects induced electrocatalytic hydrogen properties of pentagonal $\text{PdX}_2$ (X=S, Se)

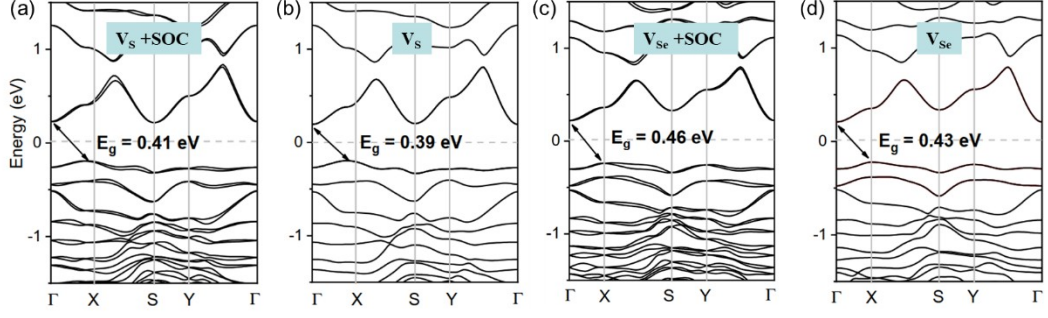
Jingjing Li,<sup>a</sup> Dan Liang,<sup>a\*</sup> Gang Liu,<sup>a\*</sup> Baonan Jia,<sup>a</sup> Jingyu Cao,<sup>a</sup> Jinbo Hao,<sup>b</sup> Pengfei Lu<sup>a</sup>

<sup>a</sup>*State Key Laboratory of Information Photonics and Optical Communications and School of Electronic Engineering, Beijing University of Posts and Telecommunications, Beijing 100876, China.*

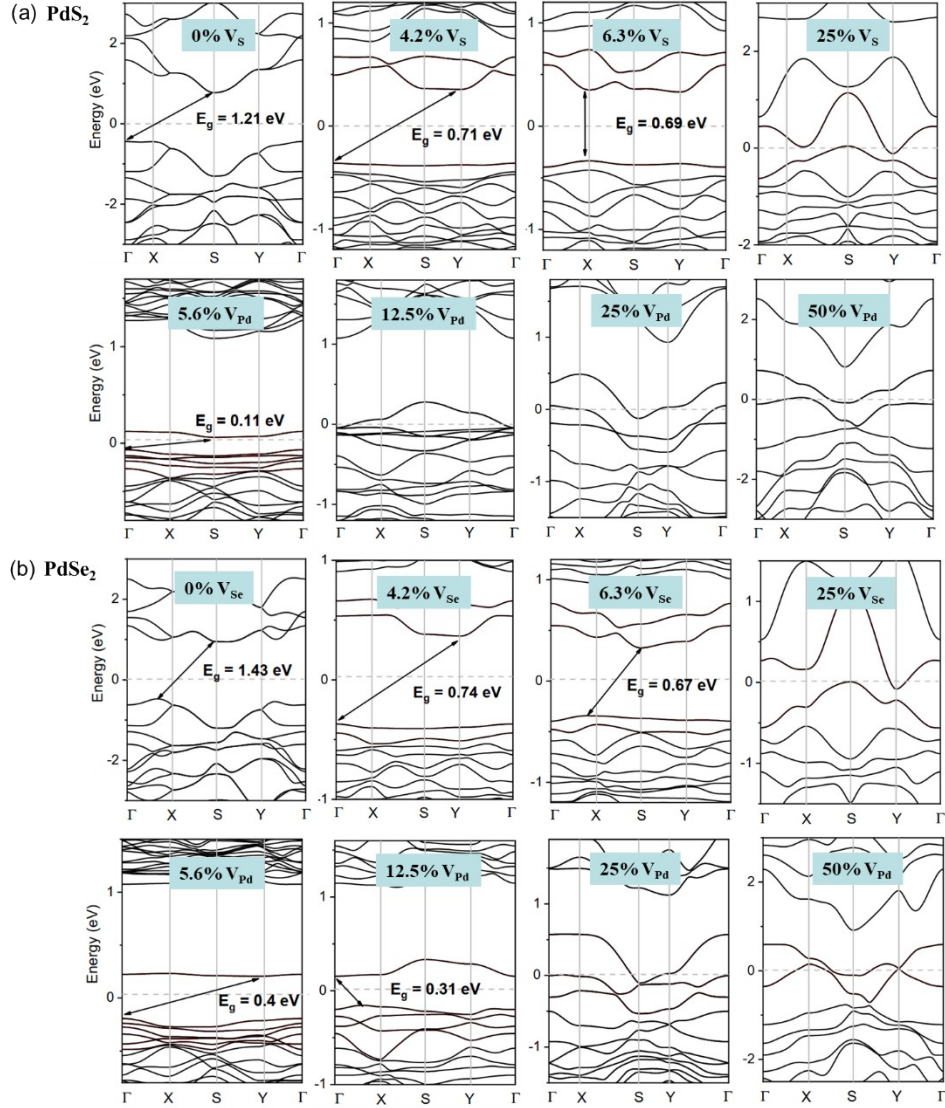
<sup>b</sup>*School of Science, Xi'an University of Architecture and Technology, Xi'an 710055, Shaanxi, China*

\*To whom correspondence should be addressed.

E-mail: [liangdan@bupt.edu.cn](mailto:liangdan@bupt.edu.cn) (D.L.), [liu\\_g@126.com](mailto:liu_g@126.com) (G.L.)



**Fig. S1.** Band structures of PdS<sub>2</sub> under 12.5%V<sub>S</sub> calculated (a) with SOC and (b) without SOC, PdSe<sub>2</sub> under 12.5%V<sub>Se</sub> calculated (c) with SOC and (d) without SOC.



**Fig. S2.** Band structures of (a) PdS<sub>2</sub> and (b) PdSe<sub>2</sub> with V<sub>S/Se</sub> and V<sub>Pd</sub> under different vacancy concentrations.