

## **The van der Waals CdO/PtS<sub>2</sub> heterostructures for photocatalytic water splitting with excellent carrier separation and light absorption**

Iqtidar Ahmad<sup>a</sup>, Ismail Shahid<sup>b</sup>, Anwar Ali<sup>c</sup>, Shakeel Zeb<sup>d</sup>, Lei Gao<sup>\*e</sup>, Jinming Cai<sup>\*a</sup>

<sup>a</sup> *School of Material Science and Engineering, Kunming University of Science and Technology, Kunming 650093, Yunnan, P. R. China. E-mail: j.cai@kust.edu.cn*

<sup>b</sup> *School of Materials Science and Engineering, Computational Centre for Molecular Science, Institute of New Energy Material Chemistry, Nankai University, Tianjin 300350, P. R. China.*

<sup>c</sup> *College of Physics and Information Technology, Shaanxi Normal University, Xian 710119, Shaanxi, P. R. China.*

<sup>d</sup> *Department of Analytical Chemistry, Institute of Chemistry, State University of São Paulo (UNESP), 14801-970 Araraquara, SP, Brazil.*

<sup>e</sup> *Faculty of Science, Kunming University of Science and Technology, Kunming 650093, Yunnan, P. R. China. E-mail: lgao@kust.edu.cn*

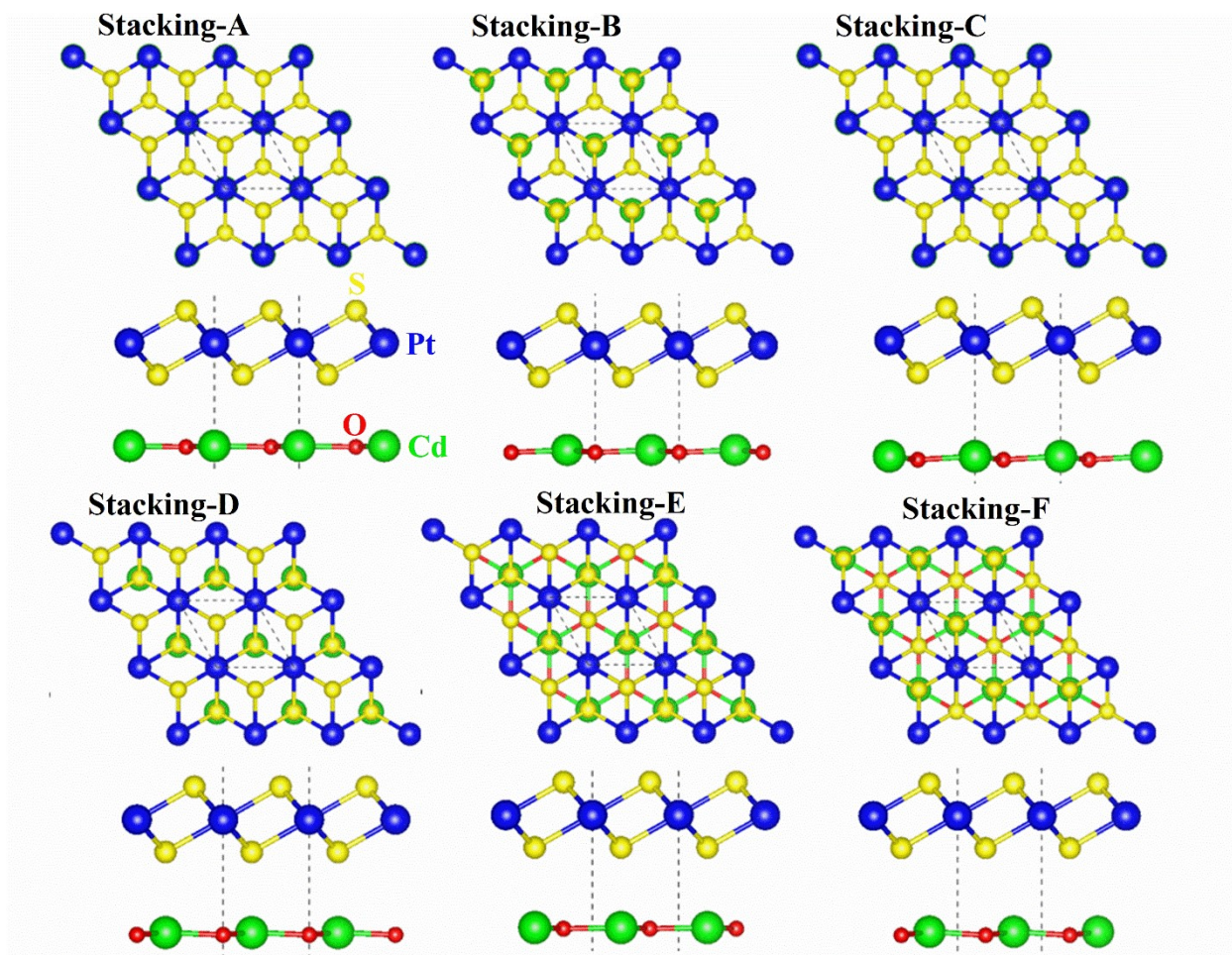


Fig. S1. All possible six patterns of CdO/PtS<sub>2</sub> heterostructures. The Cd, O, Pt and S atoms are marked by Green, red, blue and yellow colors, respectively. The dashed lines represent the primitive cell.

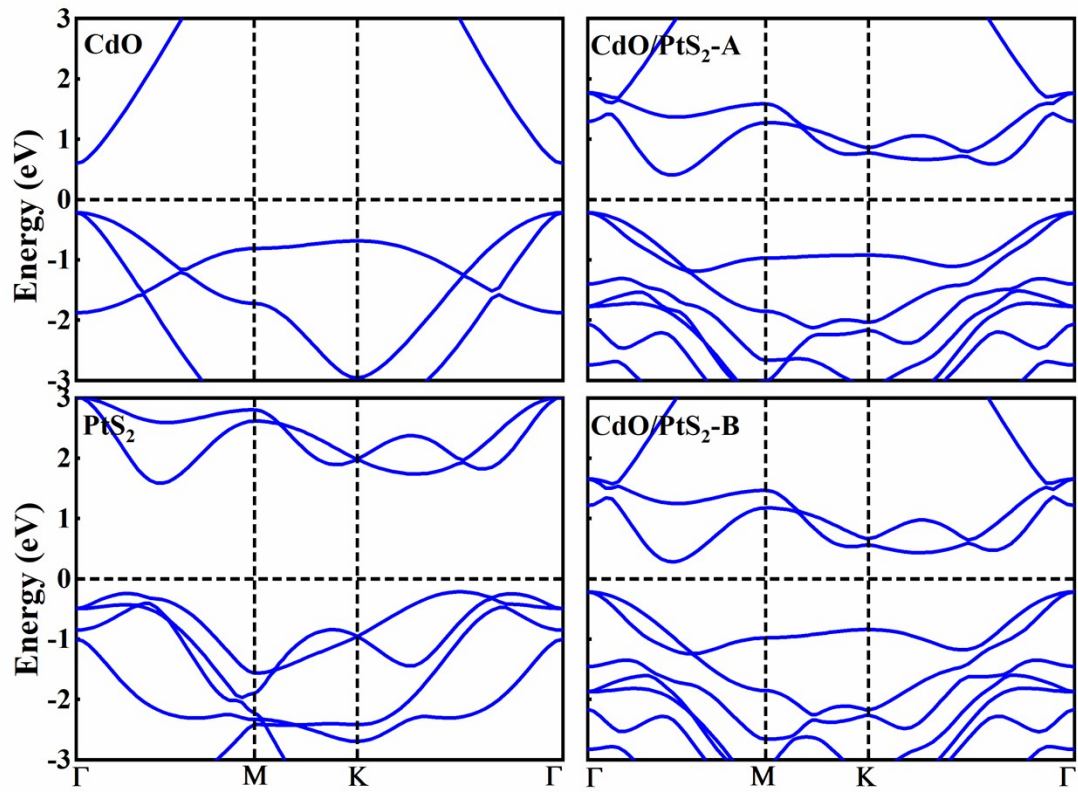


Fig. S2: The PBE band structure of pristine and their heterostructures.

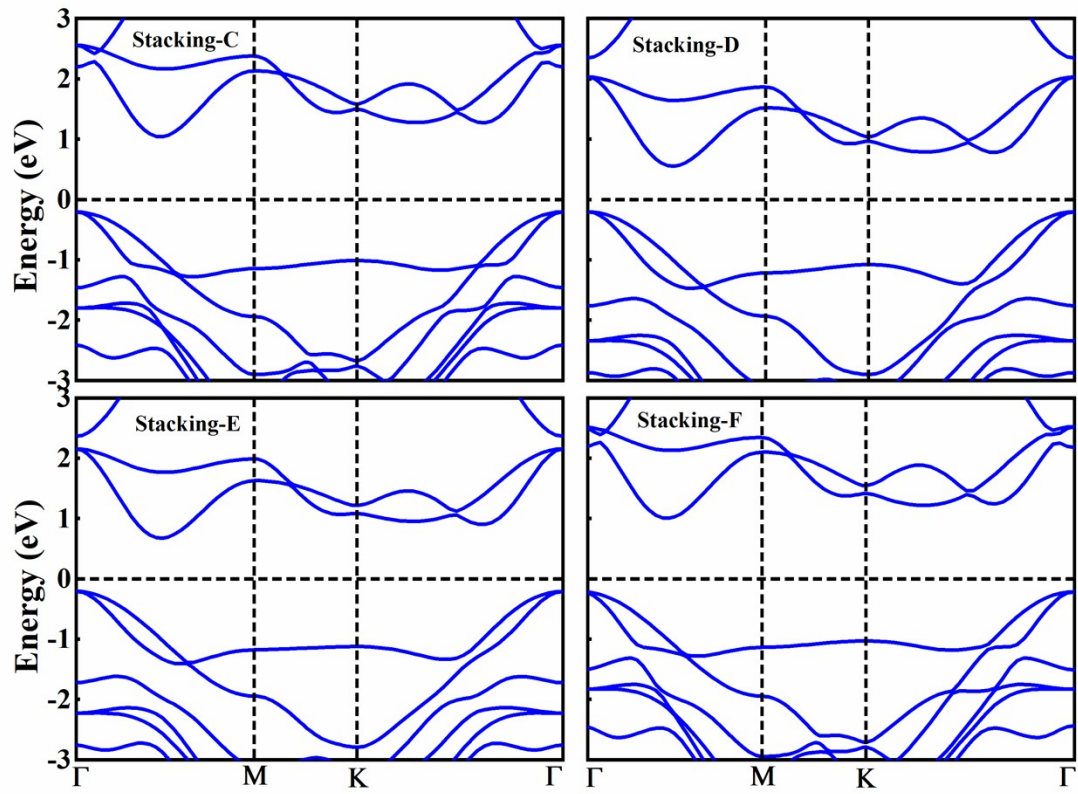


Fig. S3: The band structure of CdO/PtS<sub>2</sub> heterostructures of stacking C, D, E and F.

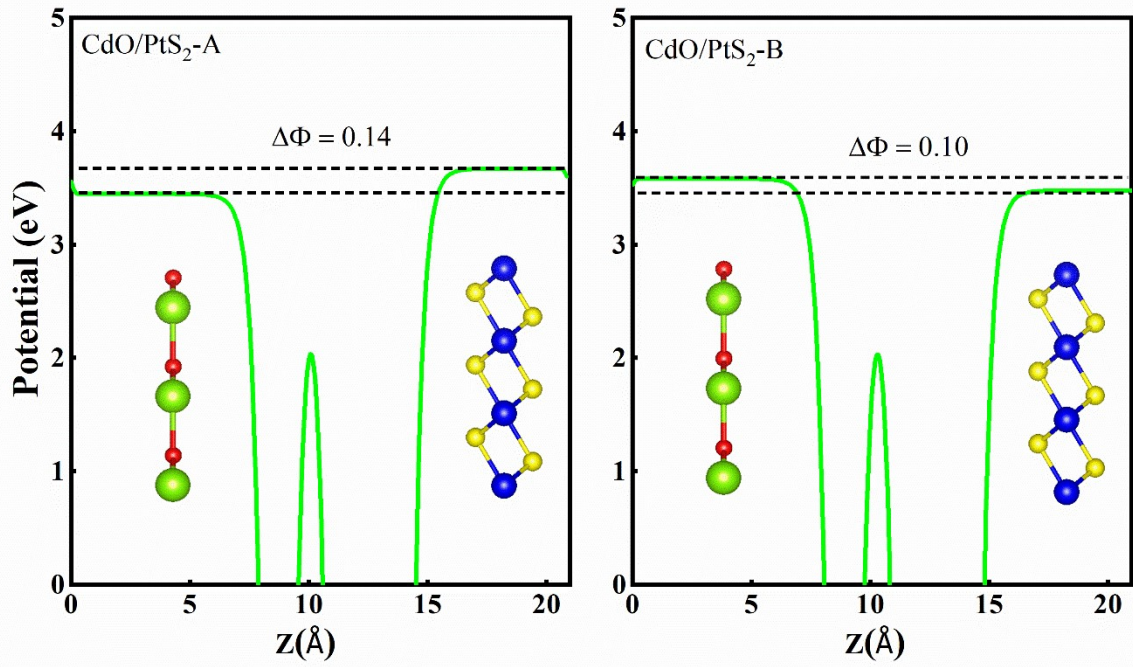


Fig. S4. The enlarged electrostatic potential of CdO/PtS<sub>2</sub>-A and CdO/PtS<sub>2</sub>-B heterostructures. The  $\Delta\Phi$  is the vacuum level difference of both sides of heterostructures.