

Mechanism of the two-dimensional WSeTe/Zr₂CO₂ direct Z-scheme van der Waals
heterojunction as photocatalysts for water splitting

Jiameng Cao,^a Xianbin Zhang,^{a*} Shihan Zhao^a, Xiaoyue Lu^a, Haohao Ma^a

Jiameng Cao (cjm@stu.xaut.edu.cn),

Xianbin Zhang (1807498999@qq.com), Shihan Zhao (unicornzsh@163.com), Xiaoyue Lu
(457764033@qq.com), Haohao Ma (mahaohao@stu.xaut.edu.cn)

ORCID Jiameng Cao:0000-0001-9215-0863

ORCID Shihan Zhao: 0000-0002-1295-2872

ORCID Haohao Ma: 0000-0003-3706-1870

^a Xi'an University of Technology, Xi'an, China

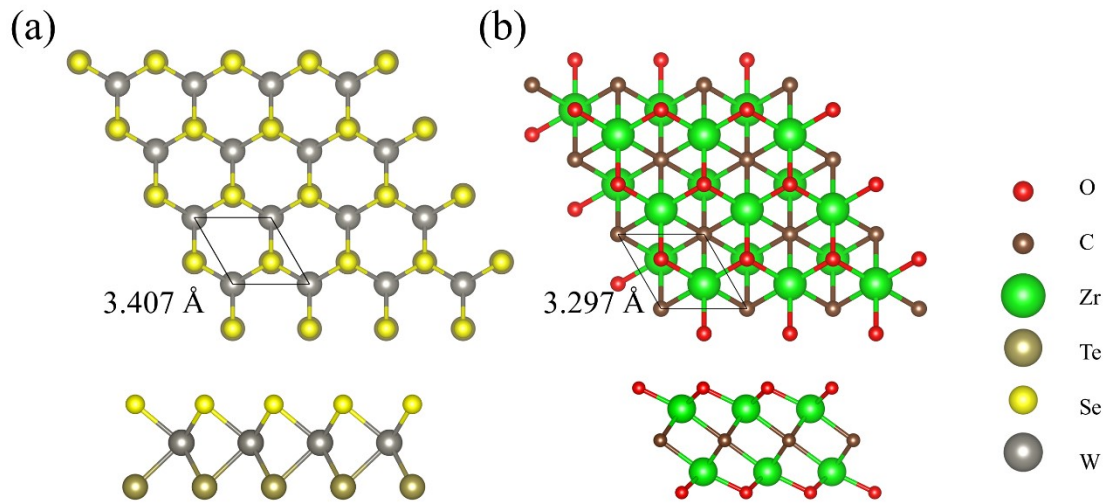


Fig. S1. Top (up) and side (down) views of optimized structures for (a) WSeTe and (b) Zr₂CO₂ monolayers. The hexagonal structures drawn by black lines represent the unit cells.

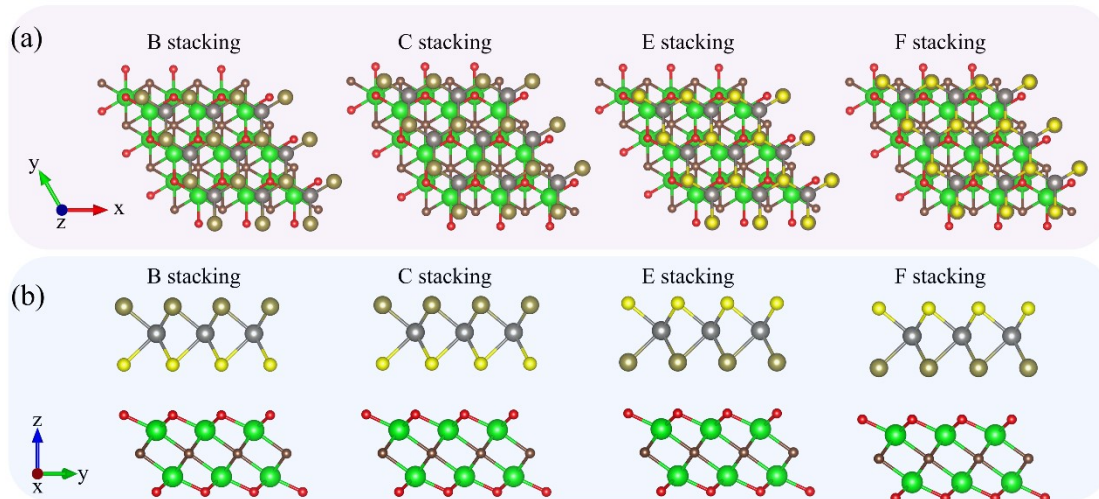


Fig. s2. Top (a) and side (b) views of the optimized structures of the WSeTe/Zr₂CO₂ heterostructure with different stacking patterns.

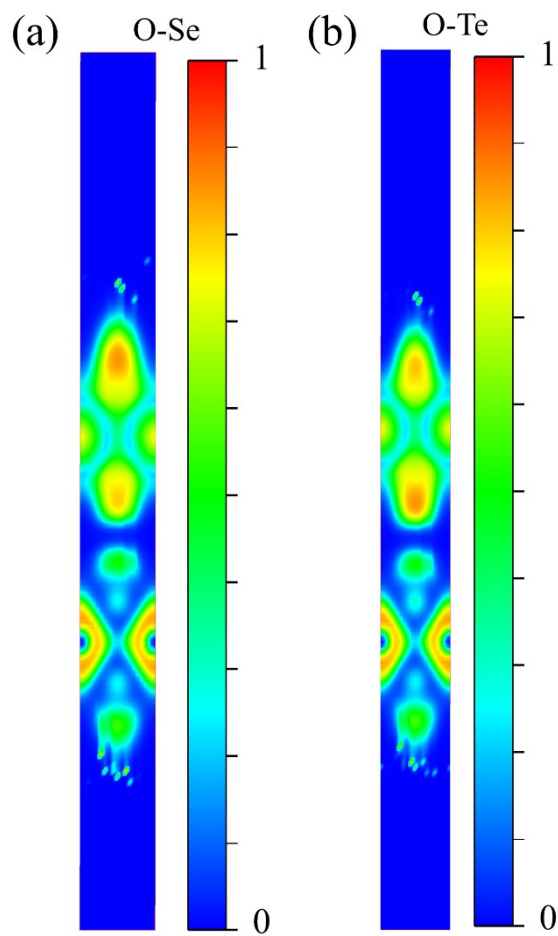


Fig. s3. Electron localization function (ELF) of WSeTe/Zr₂CO₂ vdW heterostructure of (O-Se) (a) and (O-Te) (b) model, respectively.