Electronic Supplementary Information

AlN/Ti_2CO_2 van der Waals heterostructure: a direct Z-scheme photocatalyst for efficient photocatalytic water splitting

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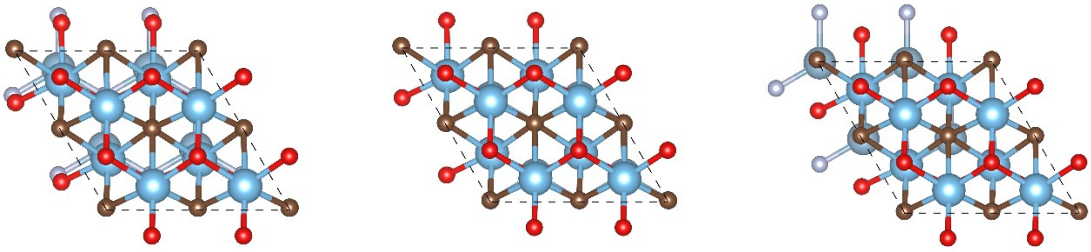


-58.7899 eV　　-58.7549 eV　　-58.6492 eV

I　　II　　III

Figure S1. The structures of AlN/Ti_2CO_2 heterostructures with different configurations and their free energies.

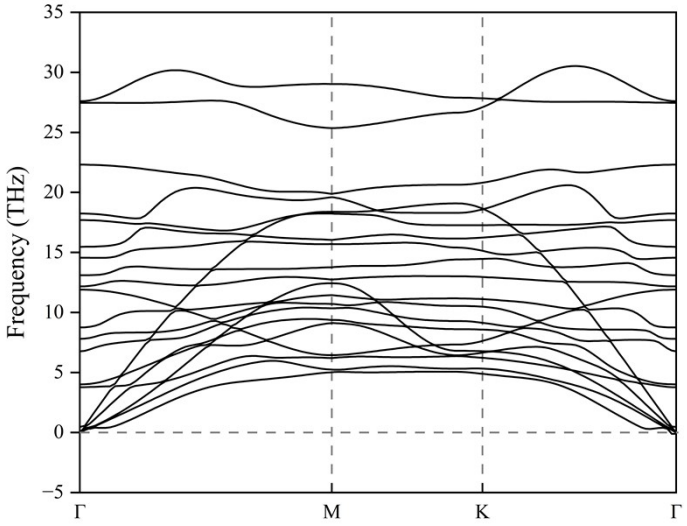


Figure S2. The phonon spectrum of AlN/Ti_2CO_2 heterostructure.

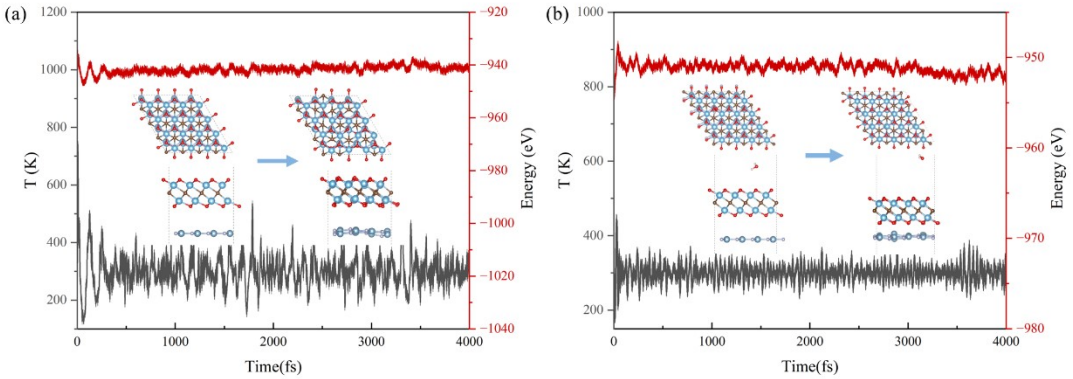


Figure S3. The fluctuations in temperature (black, left axis) and total energy (red, right axis) during AIMD simulations at 300 K for the AlN/Ti_2CO_2 heterostructure with vacancies (a) and the AlN/Ti_2CO_2 heterostructure adsorbed with water molecules (b).

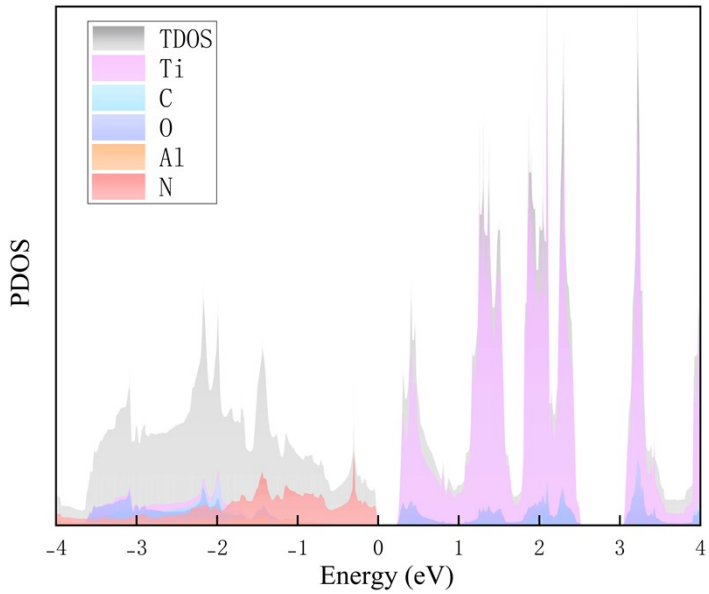


Figure S4. Projected density of states for AlN/Ti_2CO_2 heterojunctions.

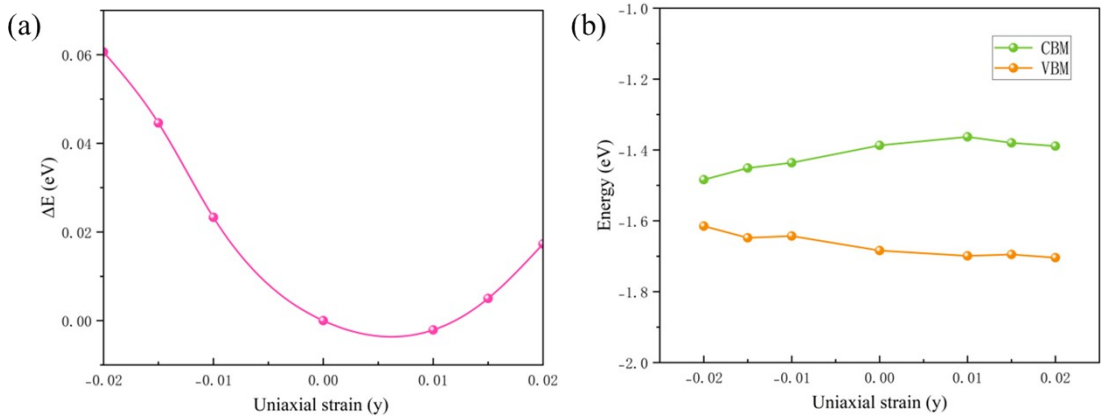
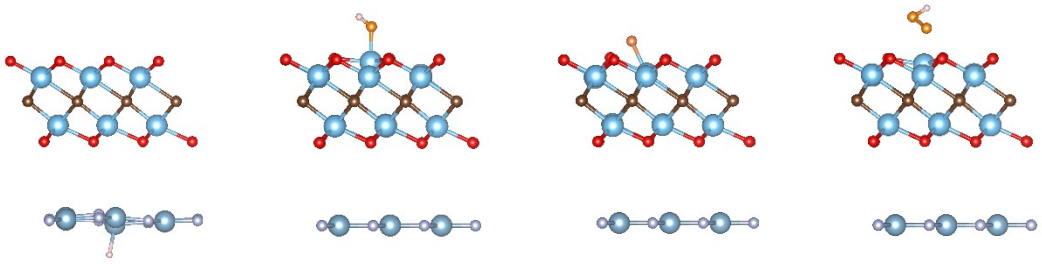


Figure S5. (a) The energy change, and (b) the band edge positions (CBM and VBM) of the heterostructures as a function of the uniaxial strain applied along y direction.



H* OH* O* OOH*

Figure S6. The intermediate structure of H*, OH*, O*, and OOH*

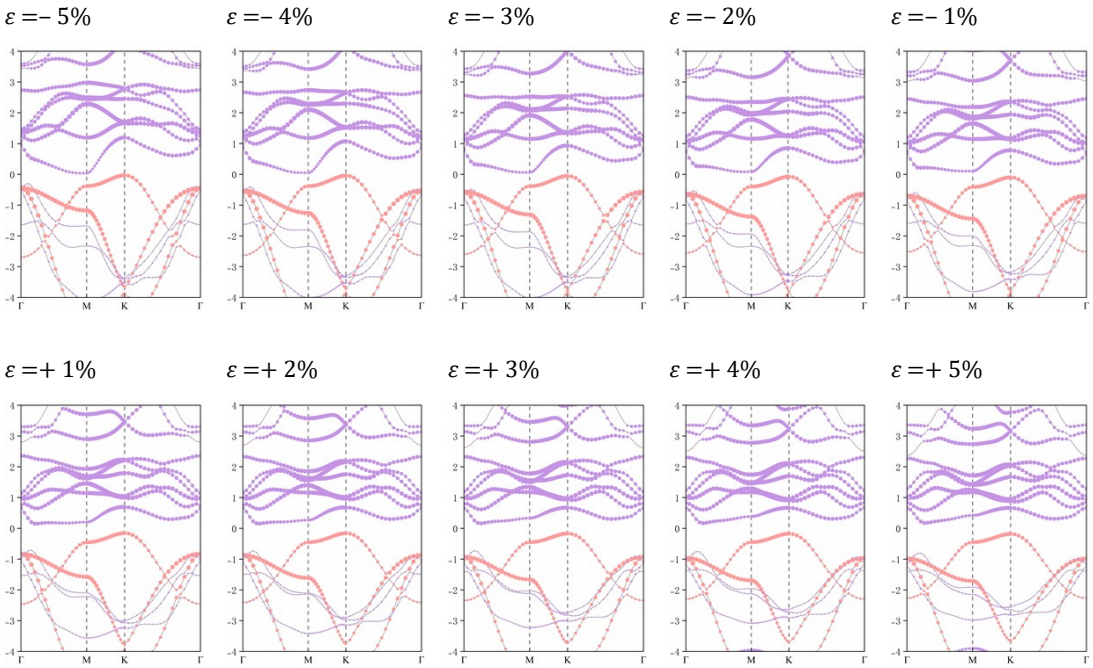


Figure S7. The band structures of the AlN/Ti_2CO_2 heterojunction under strains.