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C_2N/ZnSe heterostructure with type-II band alignment and excellent photocatalytic water splitting performance

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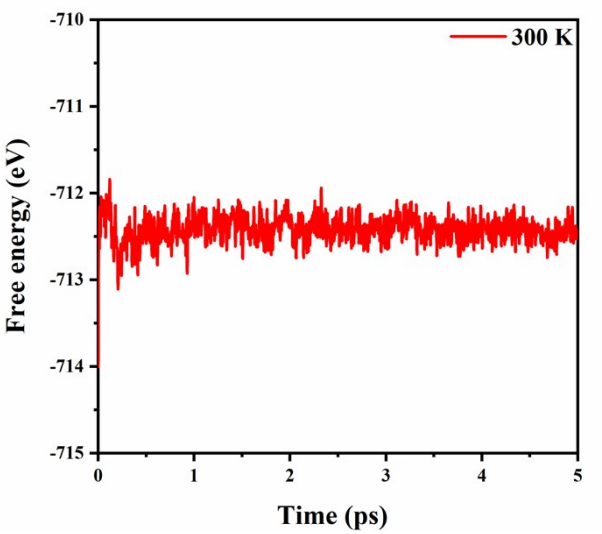

Fig. S1 (a) AIMD fluctuations of the total energy for C_2N/ZnSe heterostructure at 300 K with 5ps. (b) The top and side views of final structures in AIMD simulation.

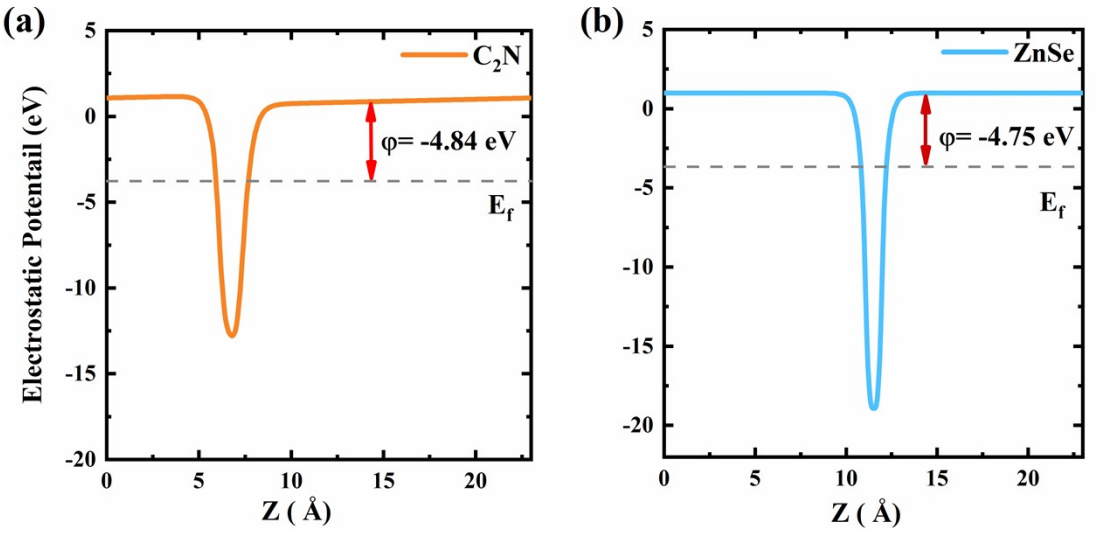

Fig. S2 Electrostatic potential of C_2N and ZnSe monolayer.

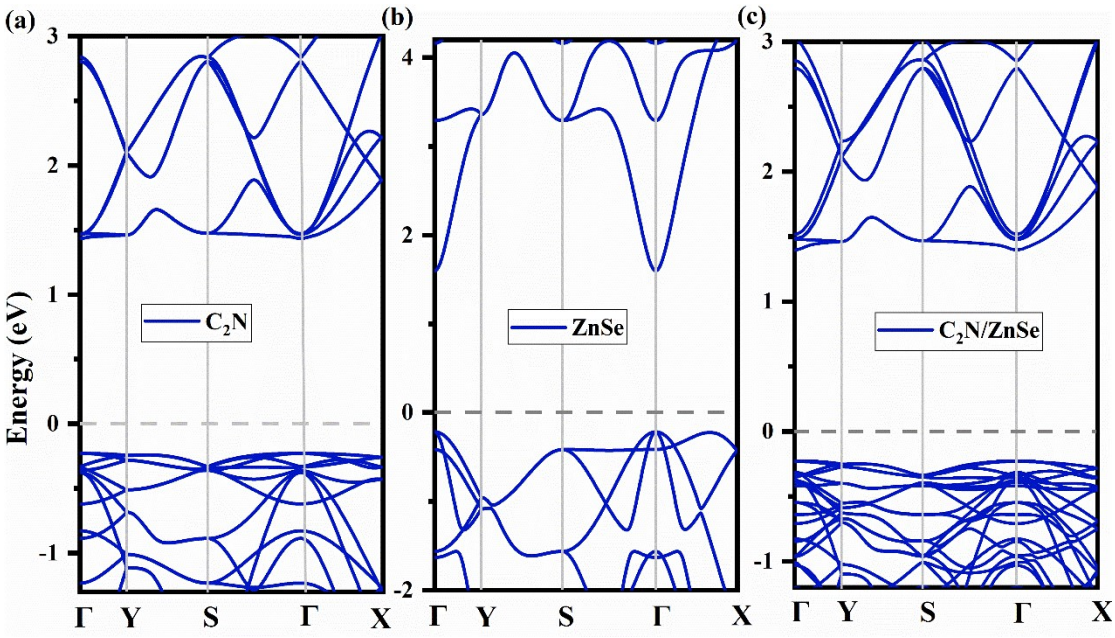

Fig. S3 Electronic band structures of (a) ZnSe monolayer, (b) C_2N monolayer and (c) C_2N/ZnSe heterostructure.

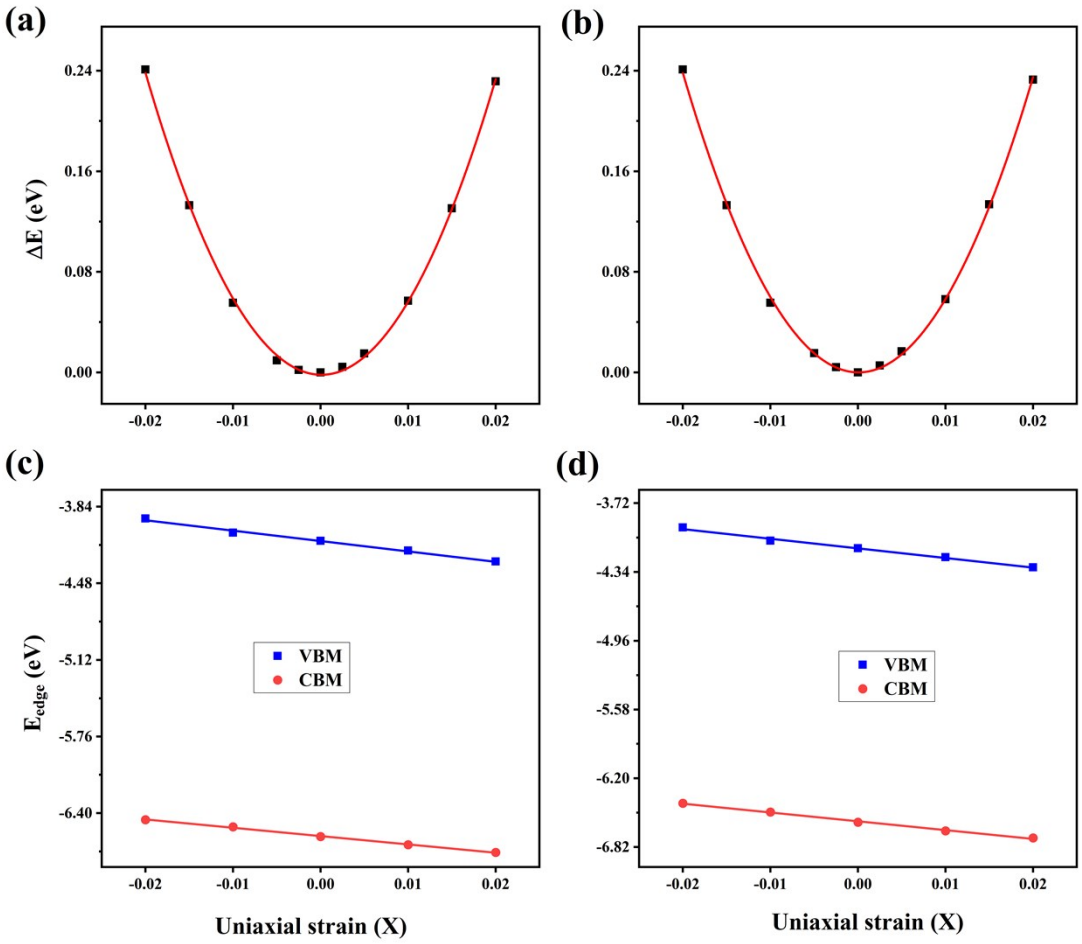

Fig. S4 (a) and (b) Engineering energy difference of monolayer C_2N as function of the uniaxial strain. (c) and (d) Band edge positions of monolayer C_2N as function of uniaxial strain along x and y directions.

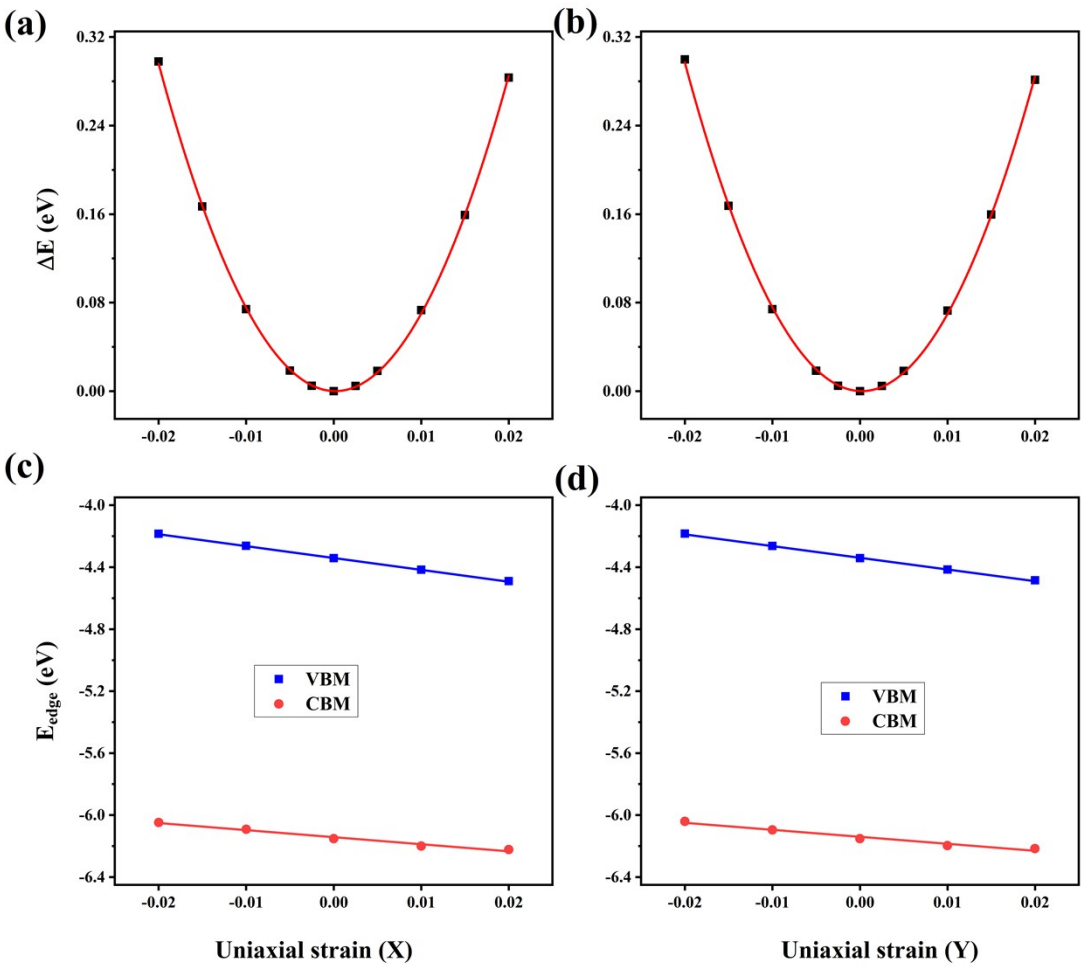

Fig. S5 (a) and (b) Engineering energy difference of monolayer ZnSe as function of the uniaxial strain. (c) and (d) Band edge positions of monolayer ZnSe as function of uniaxial strain along x and y directions.

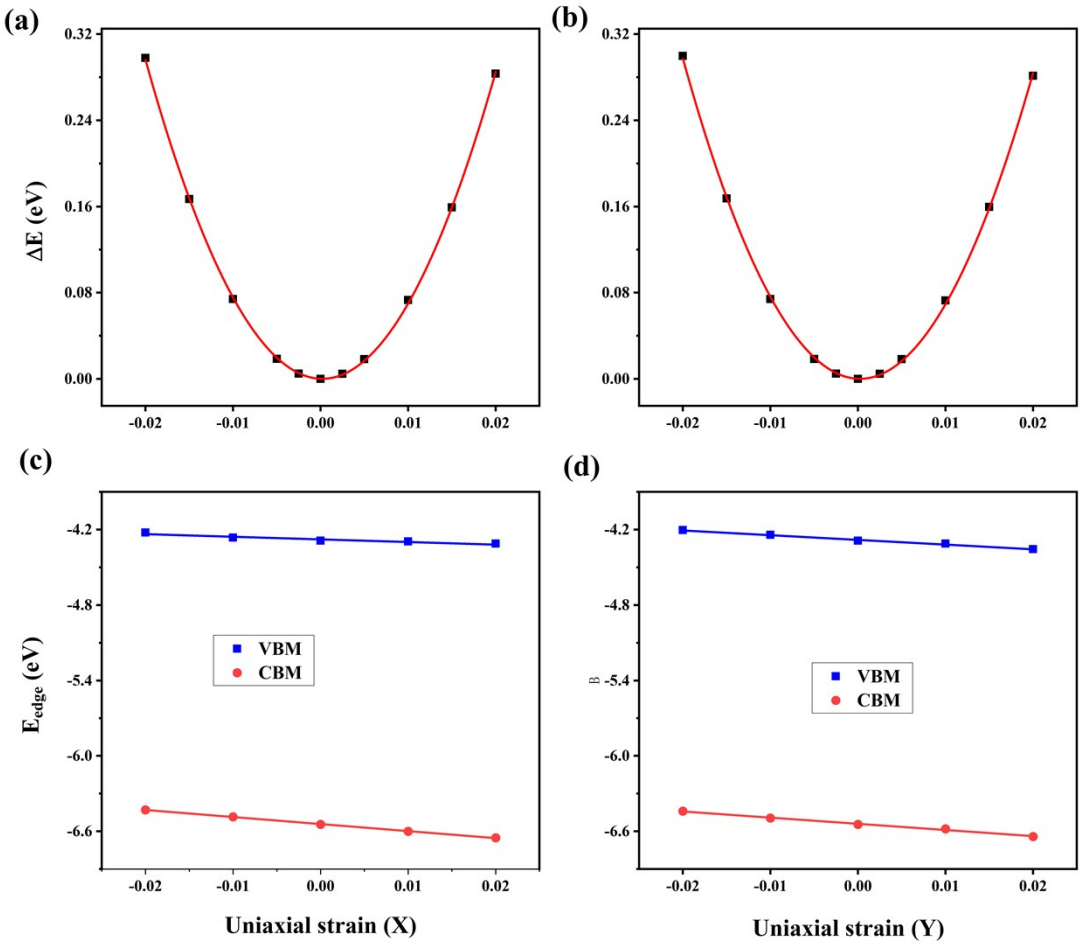

Fig. S6 (a) and (b) Engineering energy difference of monolayer C_2N/ZnSe heterostructure as function of the uniaxial strain. (c) and (d) Band edge positions of monolayer C_2N/ZnSe heterostructure as function of uniaxial strain along x and y directions.