Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Enhancement in photocatalytic water splitting using van der Waals heterostructure materials based on penta-layers

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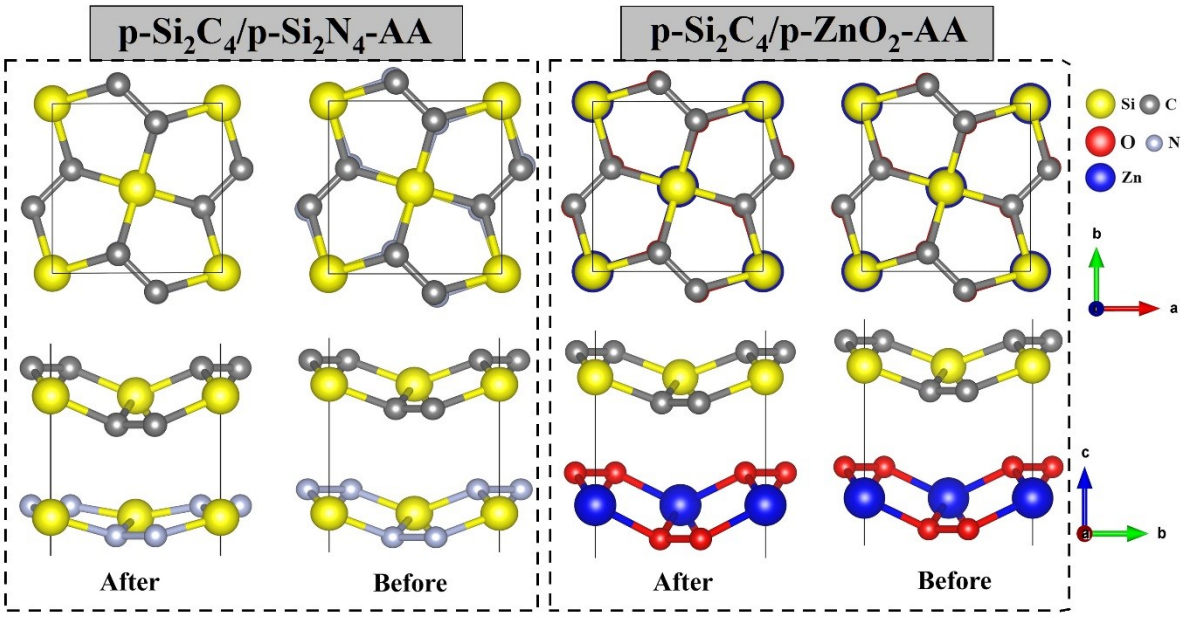

Fig. S1. Top and side views of (left) p-Si_2C_4/p-Si_2N_4, (right) p-Si_2C_4/p-ZnO_2 *vdWHs* with AA stacking mode after and before structural optimization.

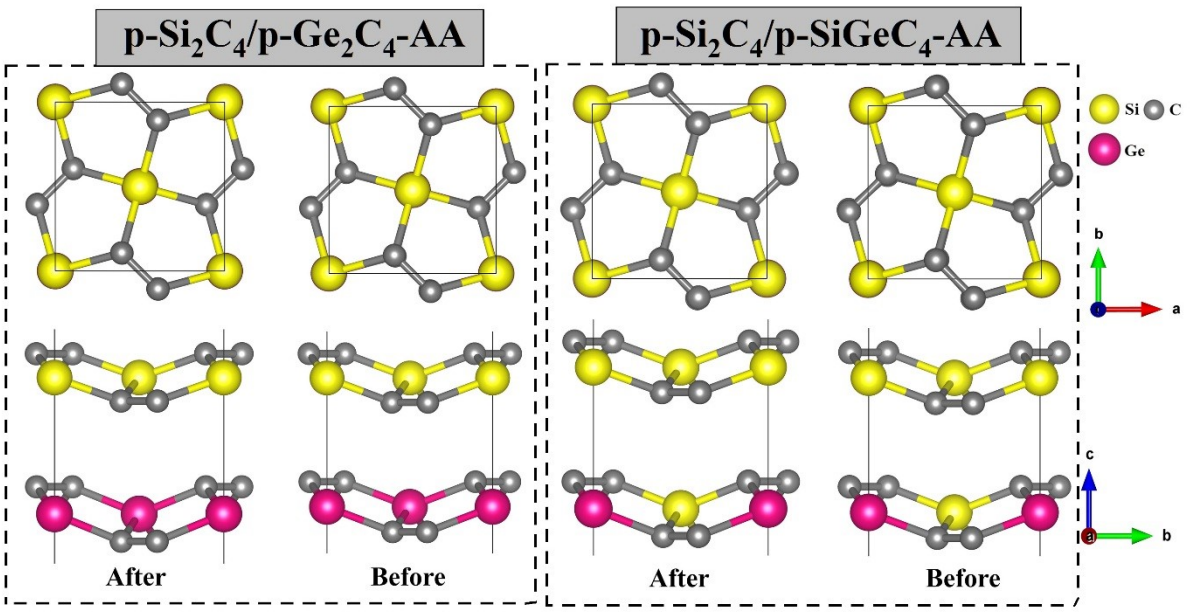

Fig. S2. Top and side views of (left) p-Si_2C_4/p-Ge_2C_4, (right) p-Si_2C_4/p-$SiGeC_4$ *vdWHs* with AA stacking mode after and before structural optimization.

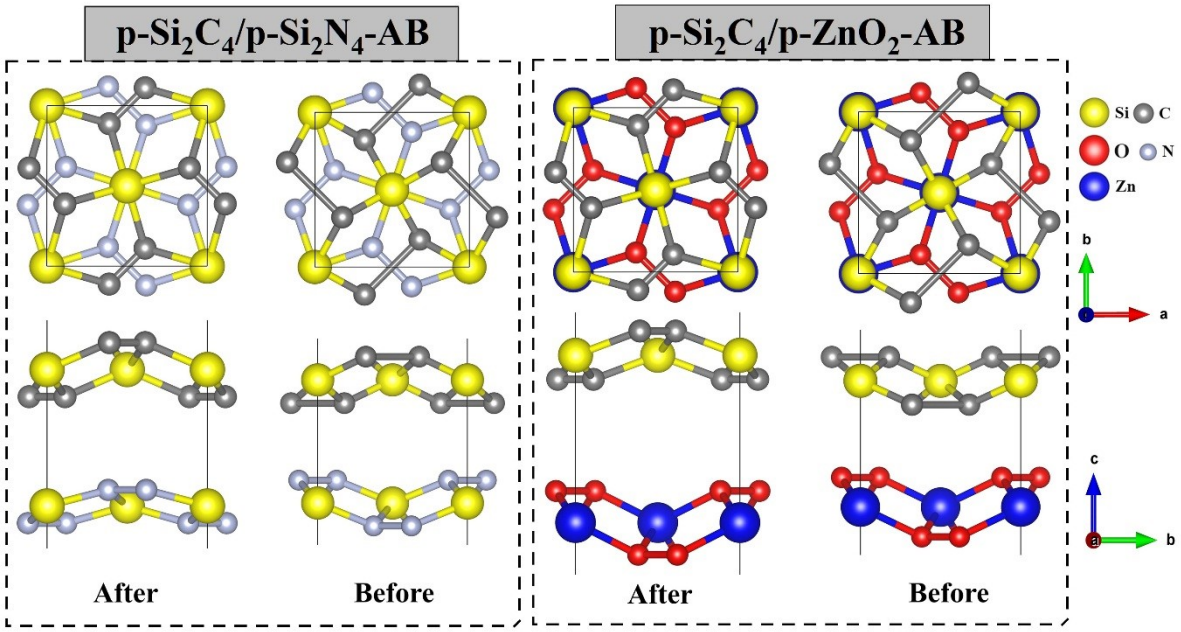

Fig. S3. Top and side views of (left) p-Si_2C_4/p-Si_2N_4, (right) p-Si_2C_4/p-ZnO_2 *vdWHs* with AB stacking mode after and before structural optimization.

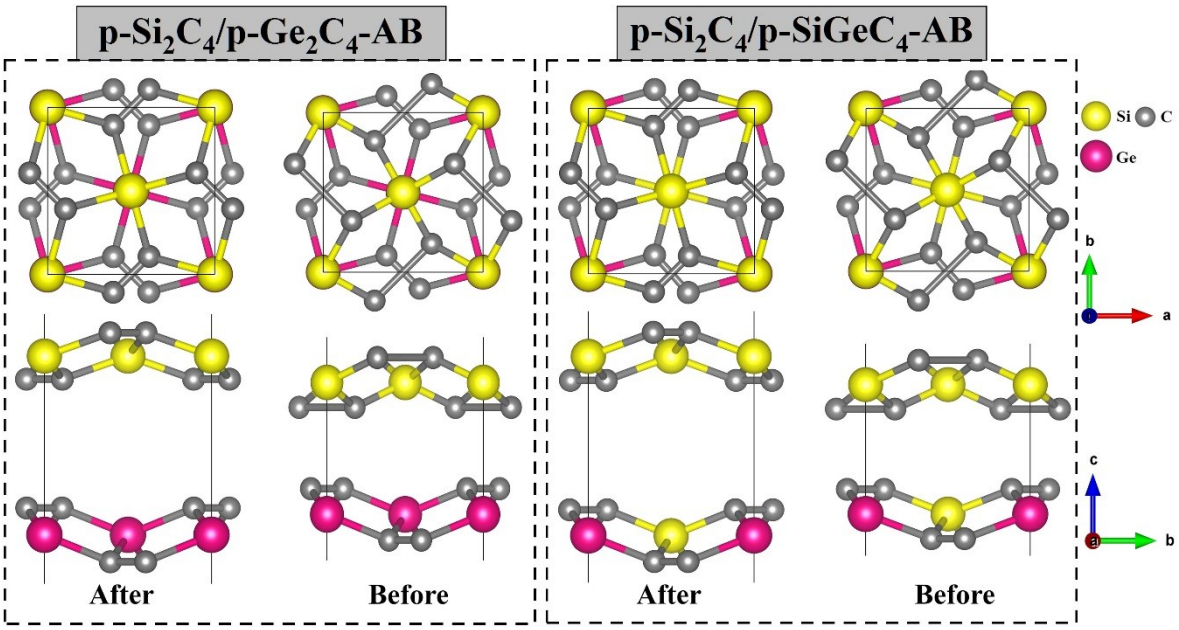

Fig. S4. Top and side views of (left) p-Si_2C_4/p-Ge_2C_4, (right) p-Si_2C_4/p-$SiGeC_4$ *vdWHs* with AB stacking mode after and before structural optimization.