Electronic Supplementary Information

Enhancing the photocatalytic hydrogen generation performance and strain regulation of the vertical GeI_2/C_2N van der Waals heterostructure: Insights from first-principles study

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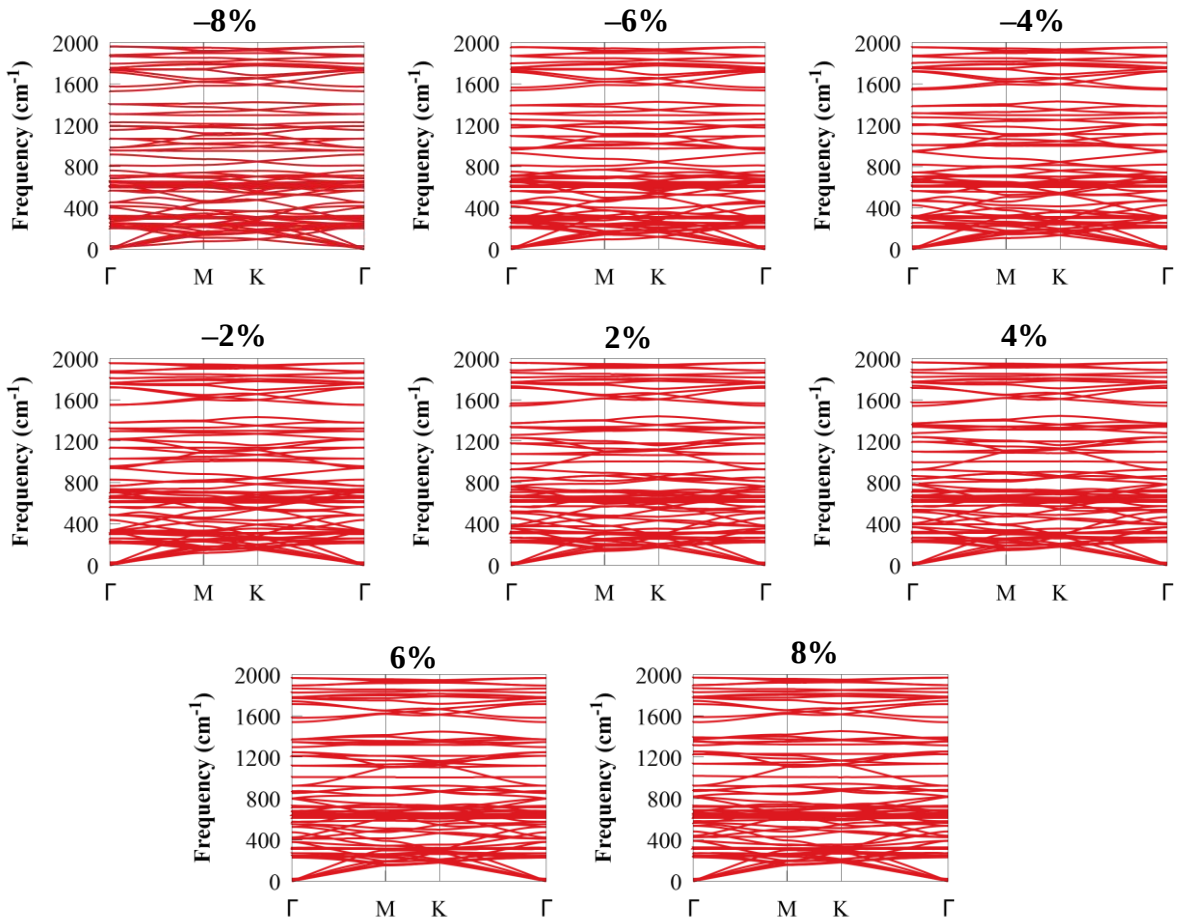

Figure S1. phonon dispersion spectra of GeI_2/C_2N vdW heterostructure under different biaxial.

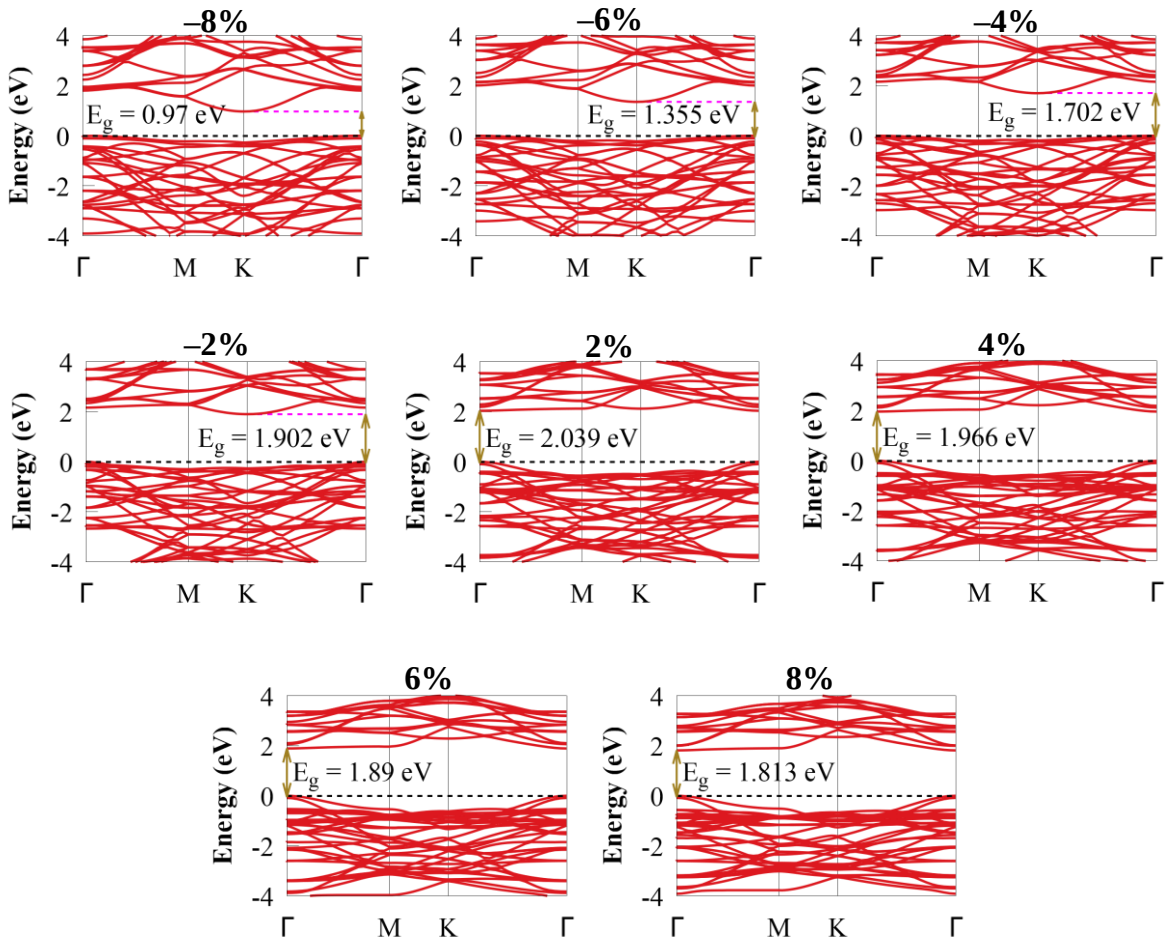

Figure S2. Electronic band structures of GeI_2/C_2N vdW heterostructure under biaxial strain. The Fermi energy is set to zero.

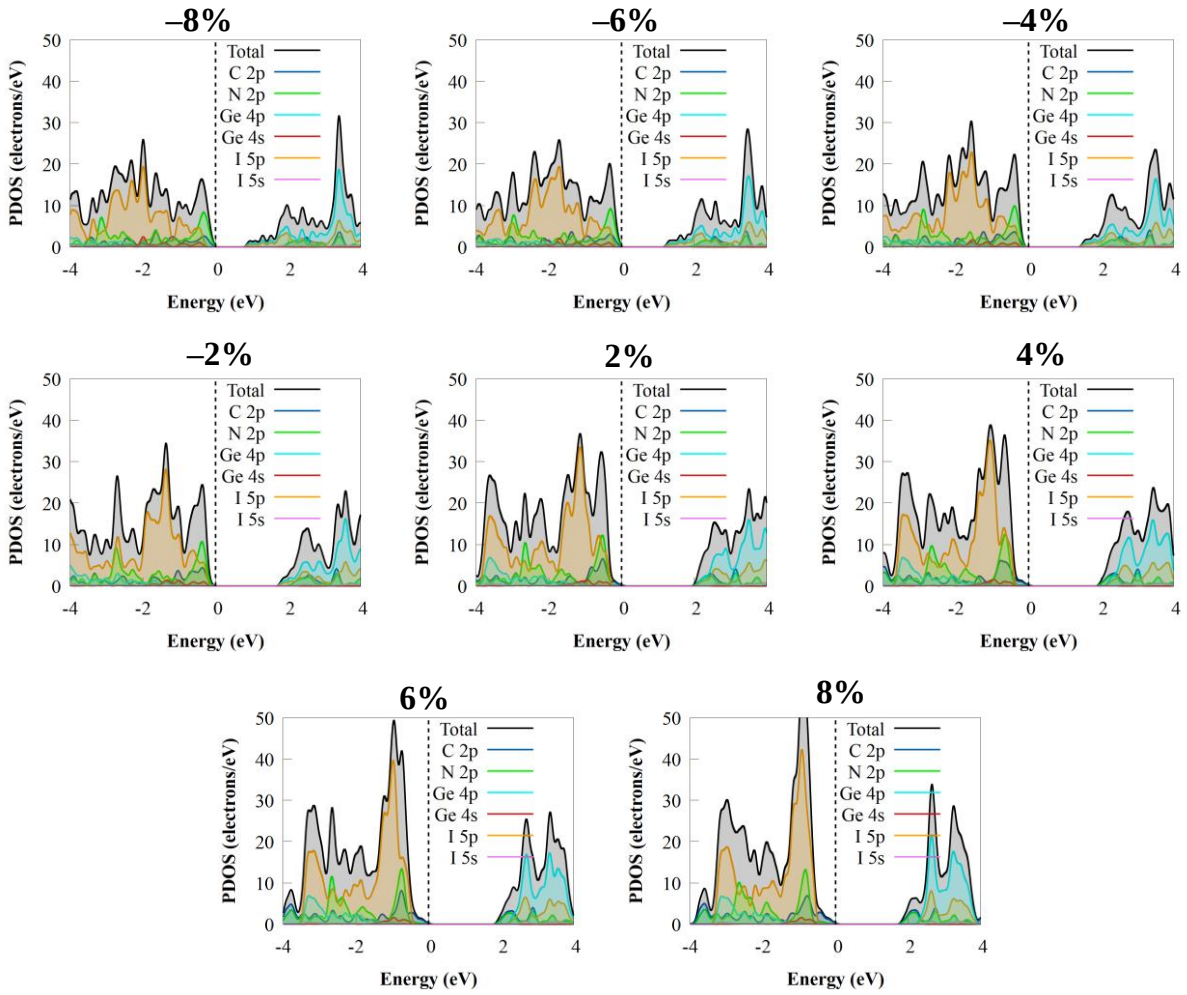

Figure S3. PDOS of GeI_2/C_2N vdW heterostructure under different biaxial strain.

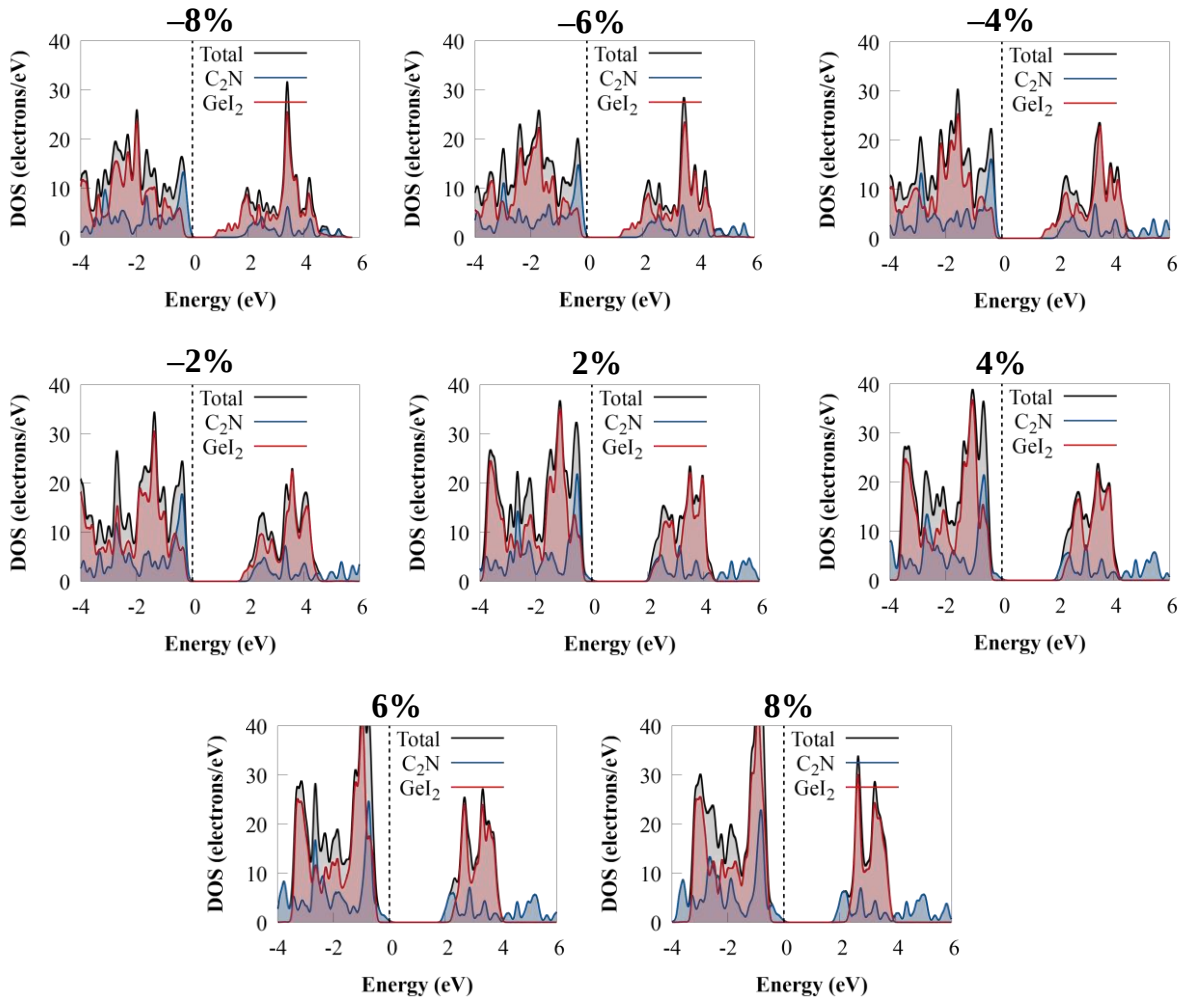

Figure S3. The calculated DOS of GeI_2/C_2N vdW heterostructure with strains of -8% to 8%. The dashed line denotes the Fermi energy level.

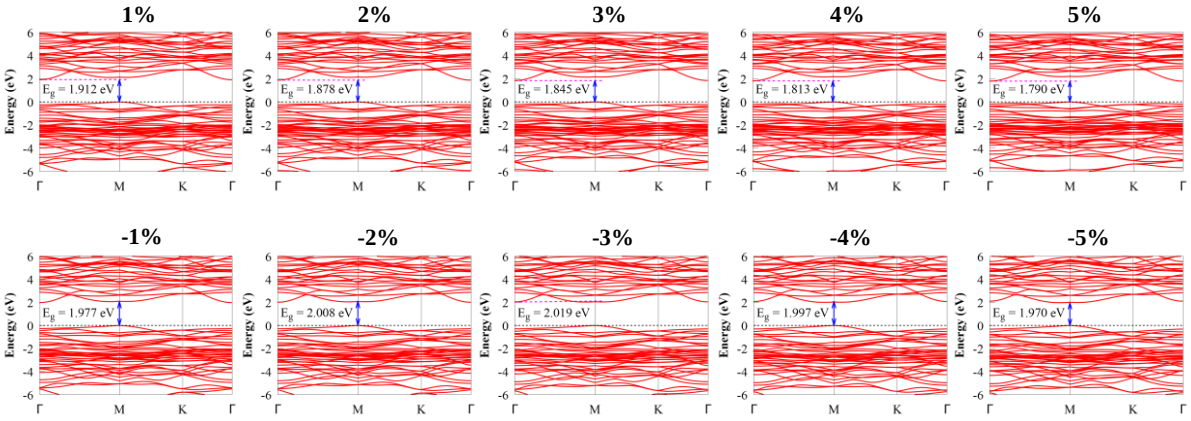

Figure S4. The band structure versus strain for HfS_2/BiOCl heterostructures