

Supporting information

Nitrogen substitution of bilayer penta-carbides: High solar-to-hydrogen and Excellent electrocatalysts for water splitting

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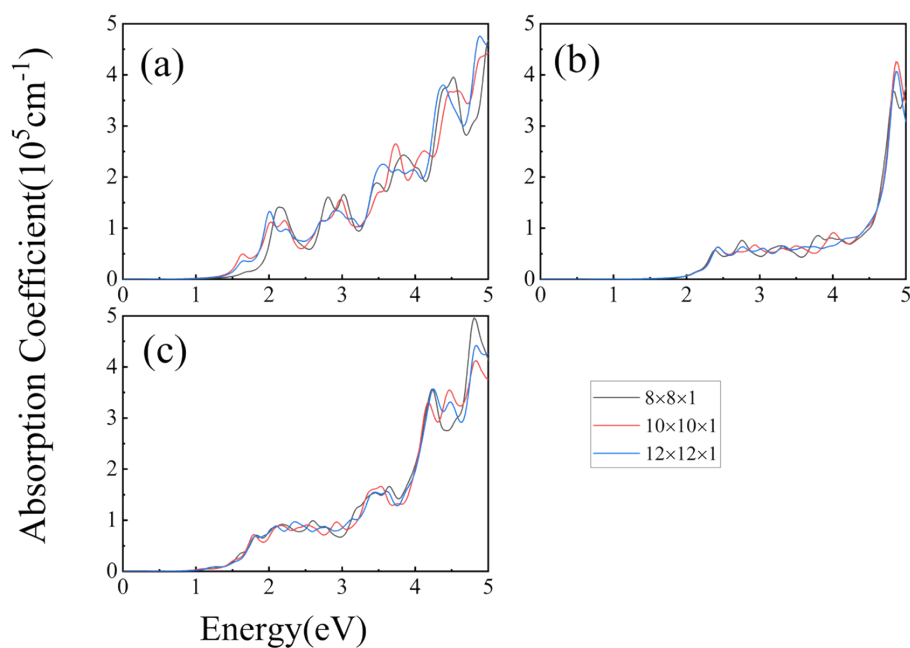


Fig. S1. K-mesh convergence test of a) $p\text{-Ge}_2\text{C}_4/\text{Ge}_2\text{N}_2\text{C}_2$, b) $p\text{-Ge}_4\text{C}_8$, c) $p\text{-Ge}_4\text{N}_4\text{C}_4$.

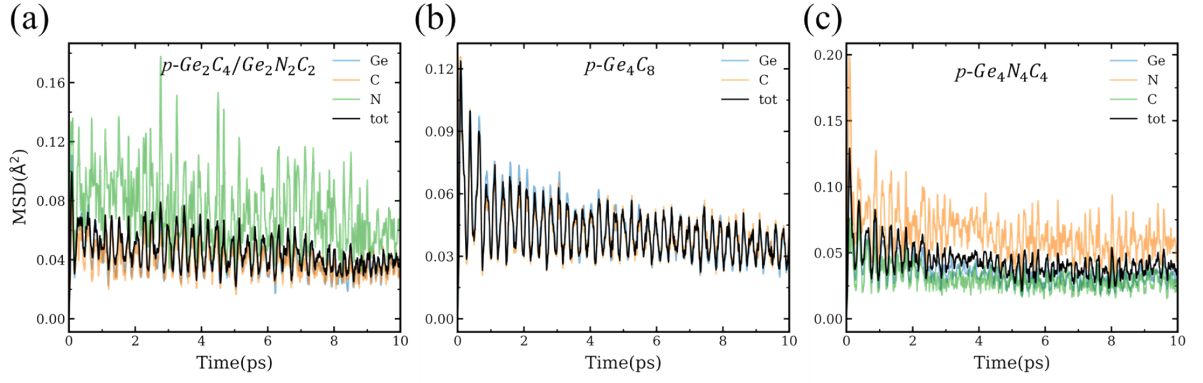


Fig. S2. The mean square displacement (MSD) of a) $p\text{-Ge}_2\text{C}_4/\text{Ge}_2\text{N}_2\text{C}_2$, b) $p\text{-Ge}_4\text{C}_8$, c) $p\text{-Ge}_4\text{N}_4\text{C}_4$.

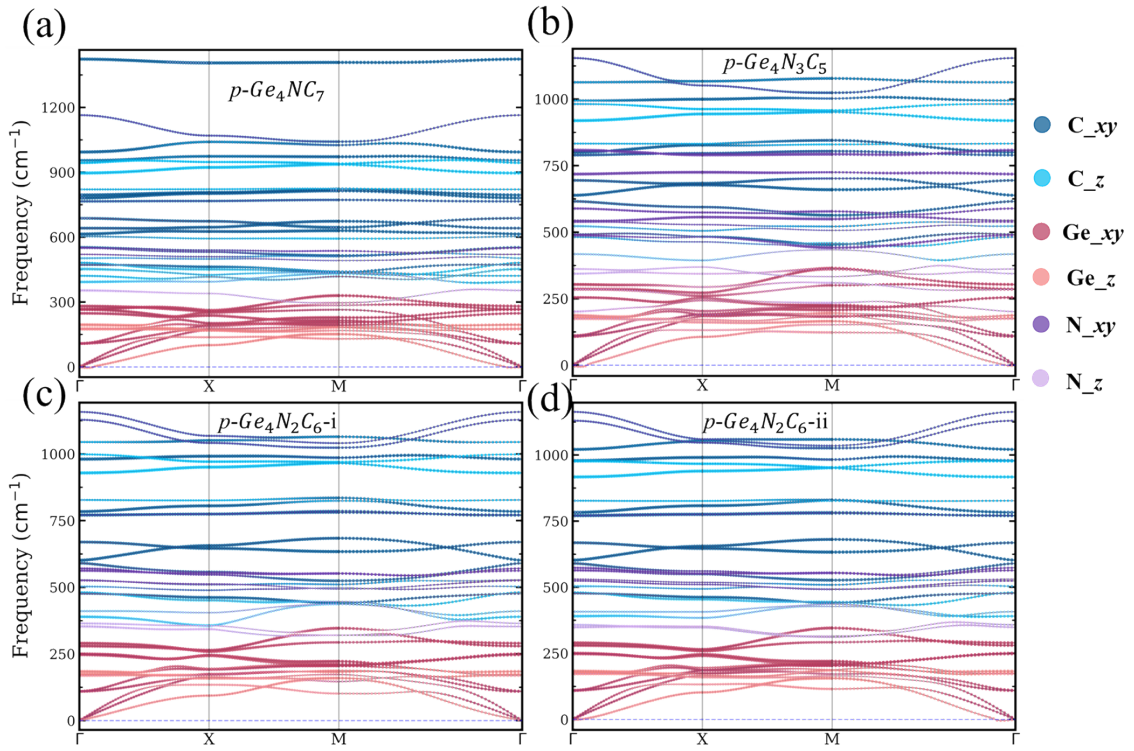


Fig. S3. Phonon dispersions of $3\times 3\times 1$ supercell of a) $p\text{-Ge}_4\text{NC}_7$, b) $p\text{-Ge}_4\text{N}_3\text{C}_5$, c) $p\text{-Ge}_4\text{N}_2\text{C}_6\text{-i}$ and d) $p\text{-Ge}_4\text{N}_2\text{C}_6\text{-ii}$.

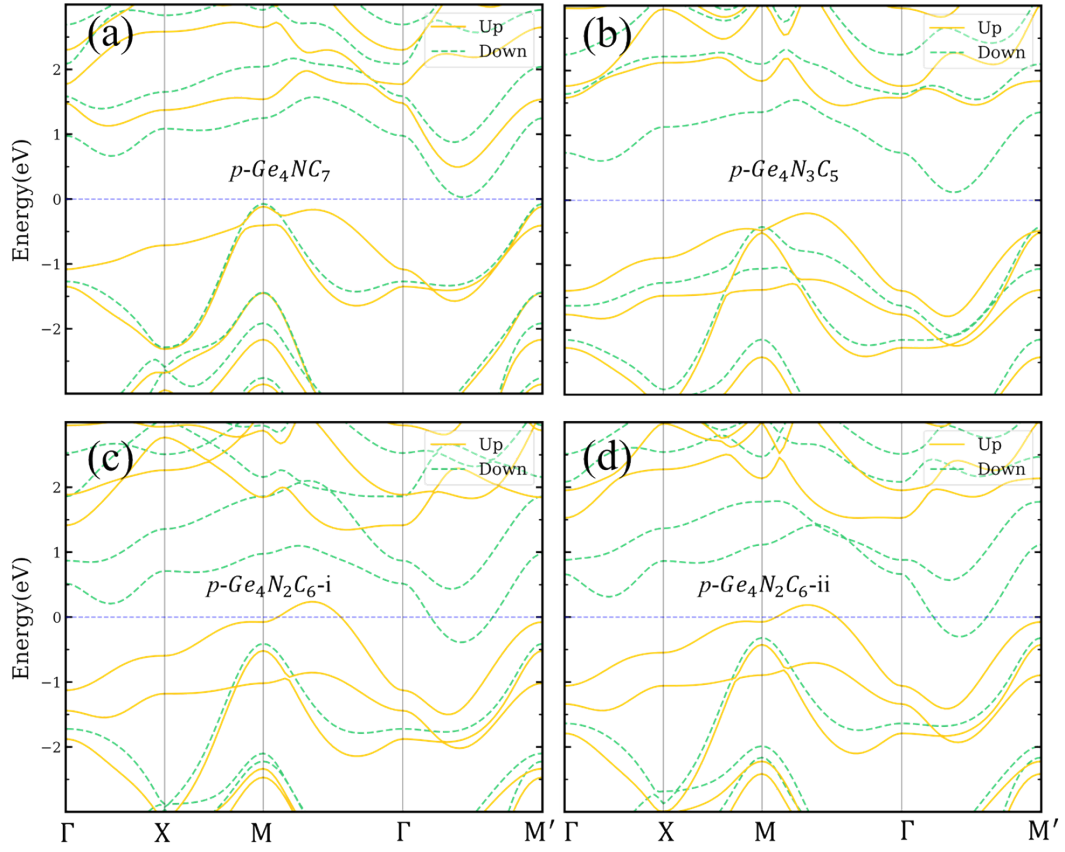


Fig. S4. Band structures of a) $p\text{-Ge}_4\text{NC}_7$, b) $p\text{-Ge}_4\text{N}_3\text{C}_5$, c) $p\text{-Ge}_4\text{N}_2\text{C}_6\text{-i}$ and d) $p\text{-Ge}_4\text{N}_2\text{C}_6\text{-ii}$ from HSE06 calculations.