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

$GaS_{0.5}Te_{0.5}$ monolayer as an efficient water splitting photocatalyst

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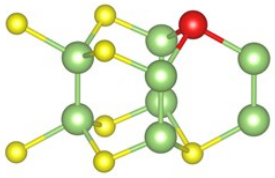
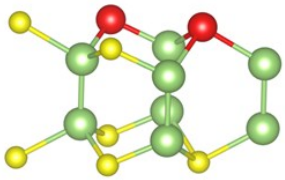
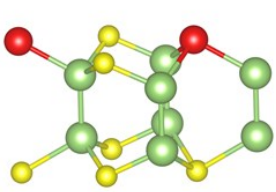
x=0.125

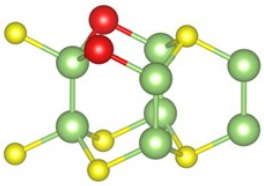


(a) -64.385959eV

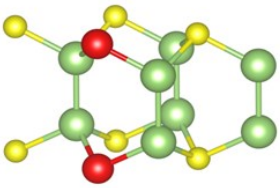
x=0.25

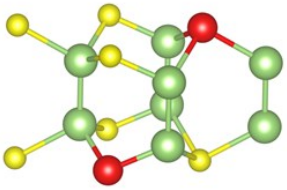




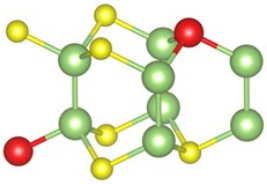


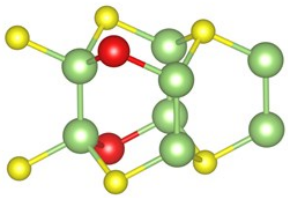
(a) -62.561162eV (b) -62.561290eV (c) -62.562420eV





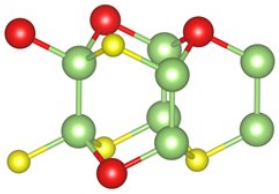
(d) -62.754536eV (e) -62.755186eV (f) -62.756198eV

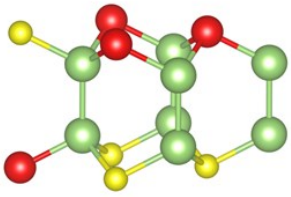




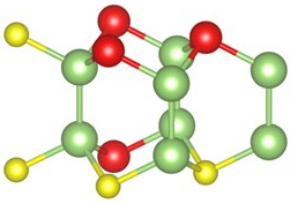
(g) -62.757681eV (h)-62.757778eV

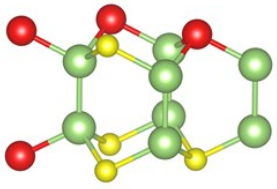
x=0.50

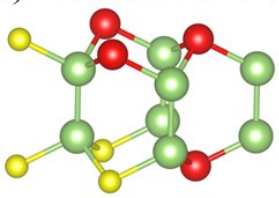




(a) -58.927825eV (b) -59.394550eV (c) -59.395804eV







(d) -59.400439eV (e) -59.401004eV (f) -59.401600eV

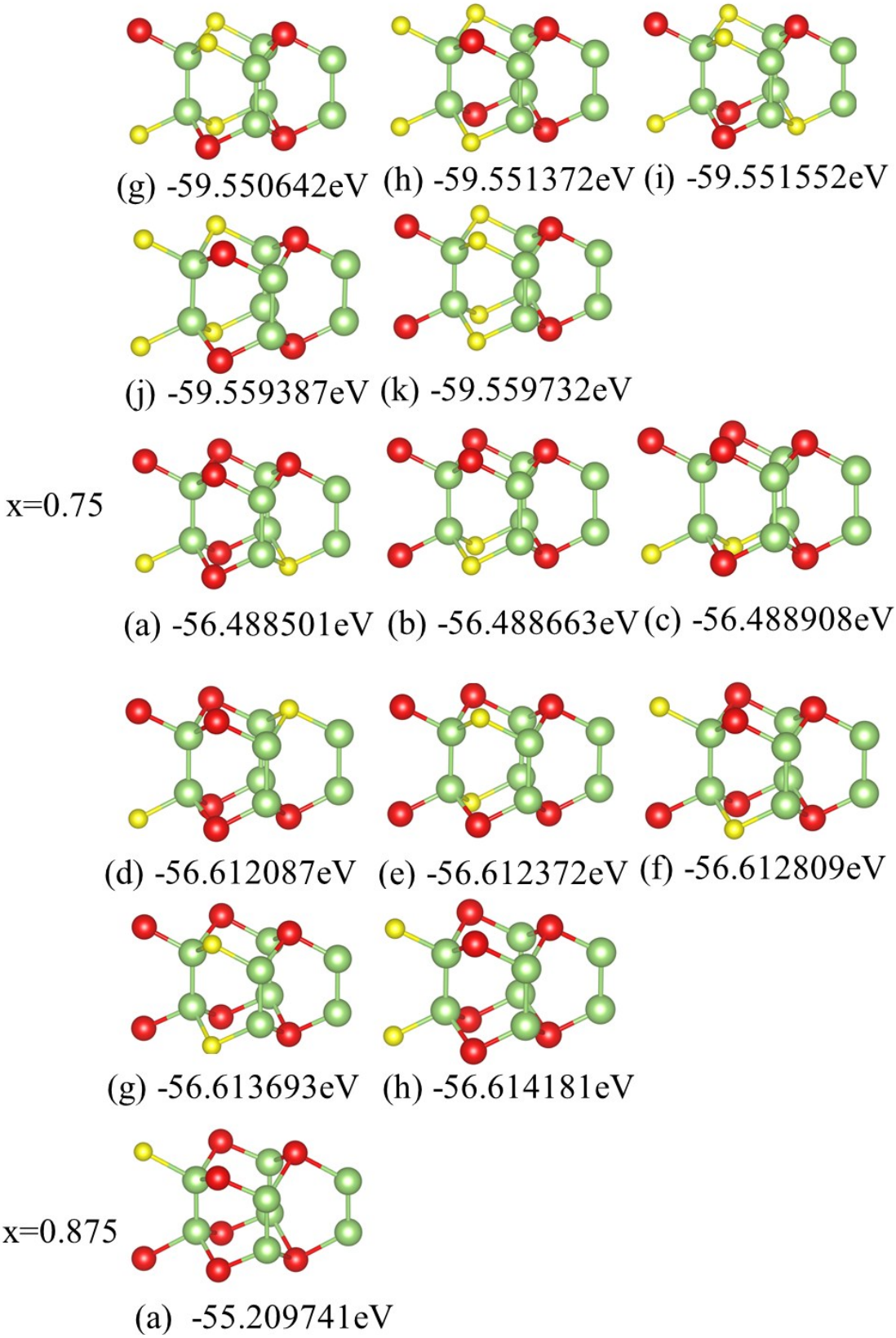


Fig.S1 shows that all calculated different configurations of substitution for x=0.125, 0.25, 0.5, 0.75, 0.875 Te doping, respectively. The calculation of the energy including zero-point energy (ZPE) corrections of each configuration is also considered.

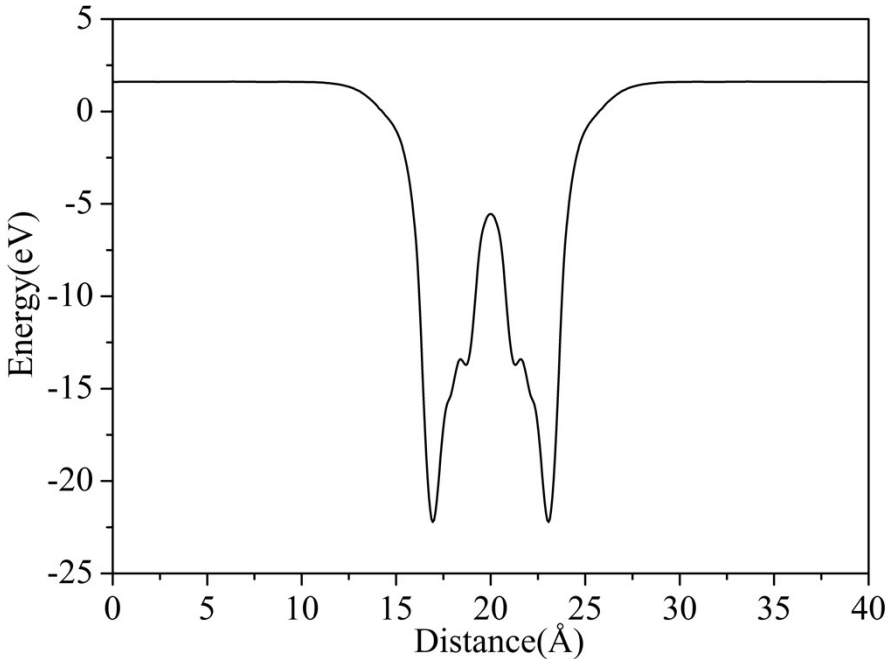


Fig.S2 shows the average electrostatic potential for GaS monolayer along the direction perpendicular to the layer calculated using the HSE06 functional. Because the calculated vacuum level by averaging the LOCPOT file from VASP is a relative value, we shift the band structure by subtracting this value to obtain the absolute position of band edge. Then we obtaine the band edge positions of the doped systems based on the extent of shifting of the CBM and VBM levels relative to that of the pristine GaS monolayer.

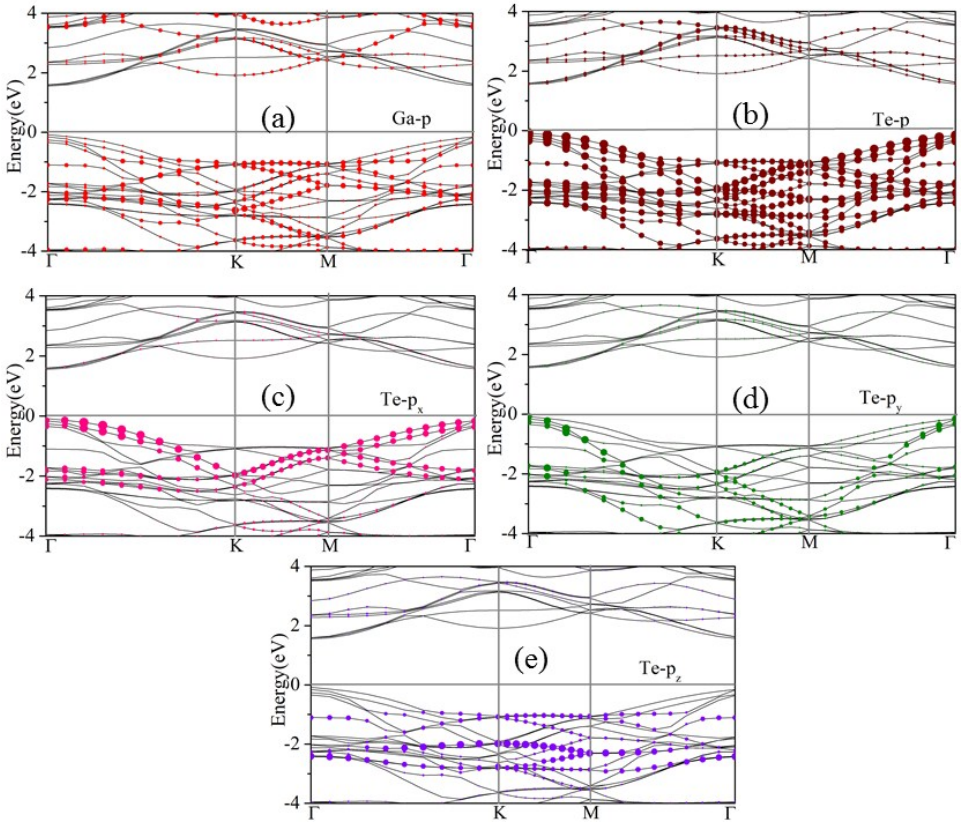


Fig.S3 Orbital decomposition of band structure for the GaTe monolayer with 6% compressive strain. The size of the circles in each band denotes the contributions from different atomic orbitals. The horizontal gray lines represent the Fermi levels.

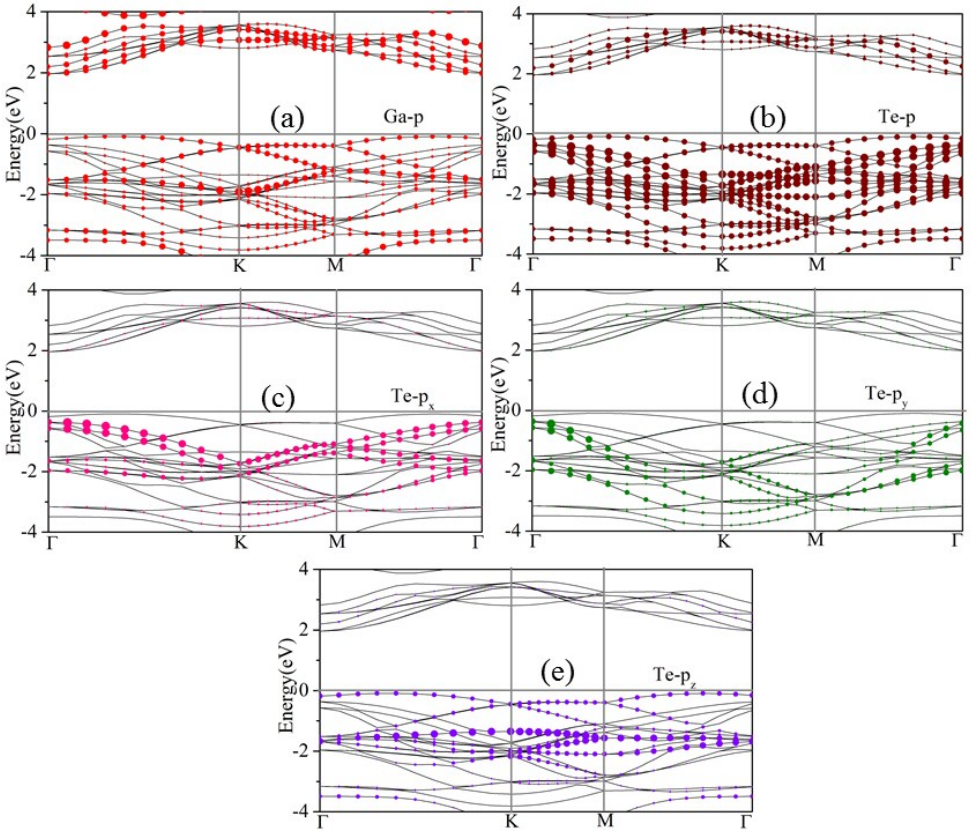


Fig.S4 Orbital decomposition of band structure for pristine GaTe monolayer. The size of the circles in each band denotes the contributions from different atomic orbitals. The horizontal gray lines represent the Fermi levels.