Supplementary Information

Tunable Electronic and Dielectric Properties of β-Phosphorene Nanoflakes for Optoelectronic Applications

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(Oct. 5, 2016)

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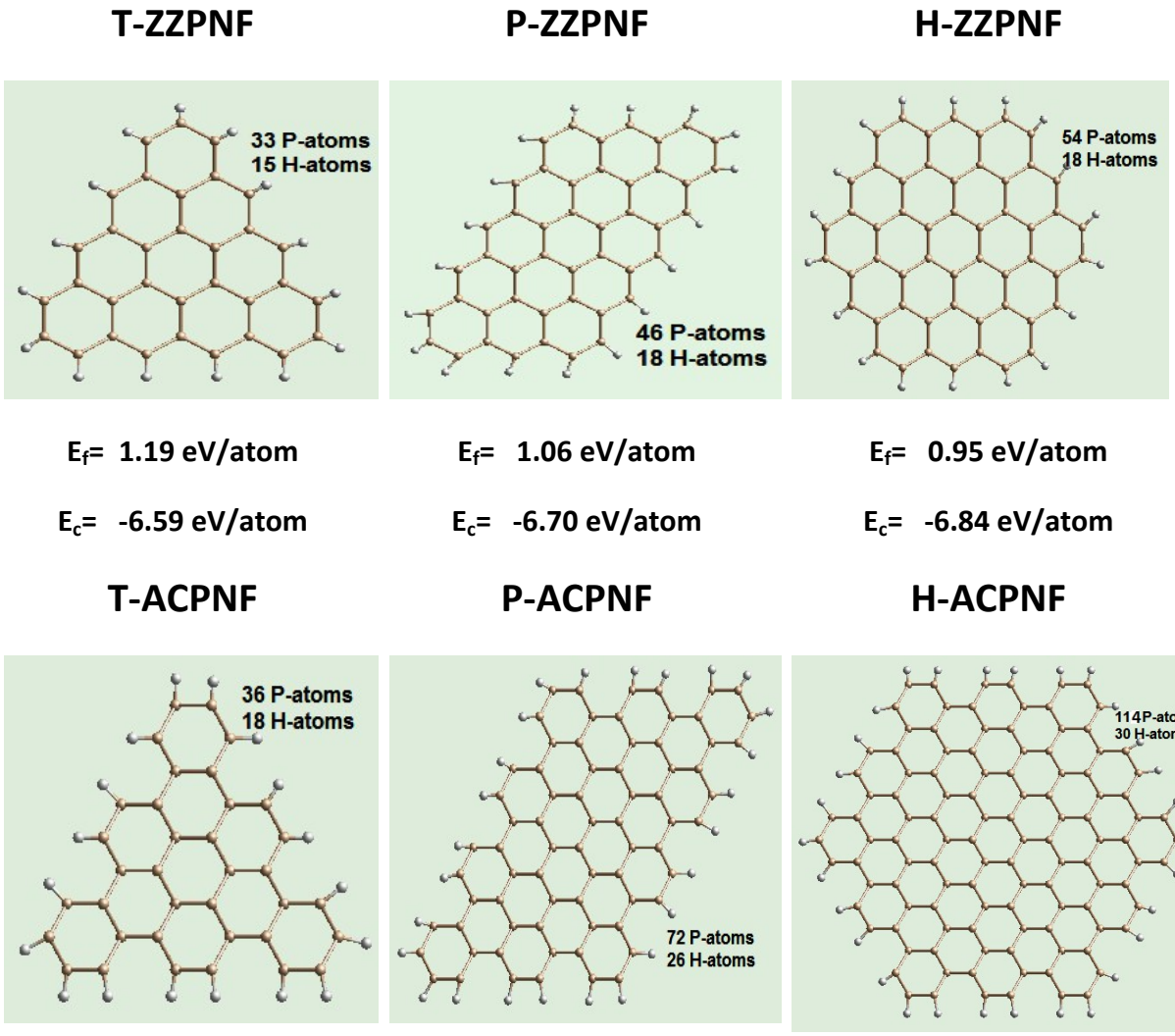

Figure S1: Various β-phosphorene hydrogen passivated nanoflakes with zigzag (ZZ) and armchair (AC) edge structures with triangular (T), parallelogram (P) and hexagonal (H) shapes. The formation energy (E_f) and cohesive energy (E_c) are also shown with each hydrogen passivated nanoflakes.

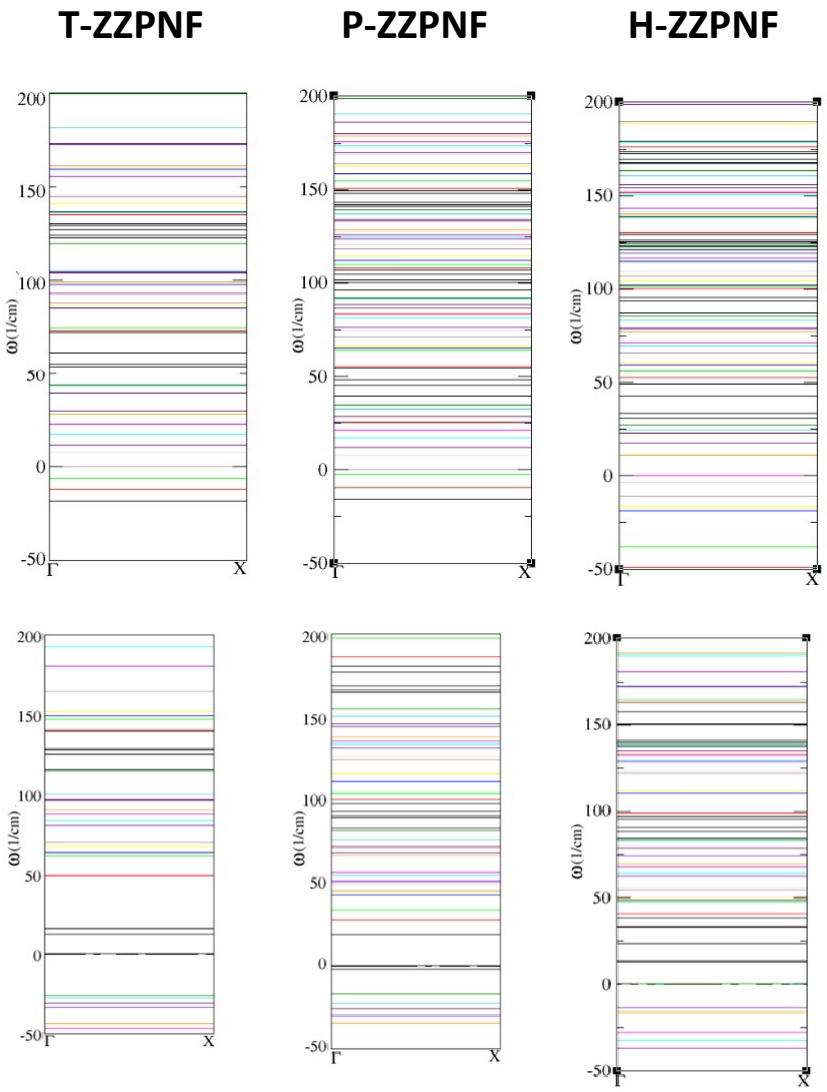

Figure S2: Phonon spectra of zigzag (ZZ) edge β-phosphorene nanoflakes with triangular (T), parallelogram (P) and hexagonal (H) shapes. Upper panel has bare ZZPNFs while lower panel has corresponding hydrogen passivated nanoflakes.

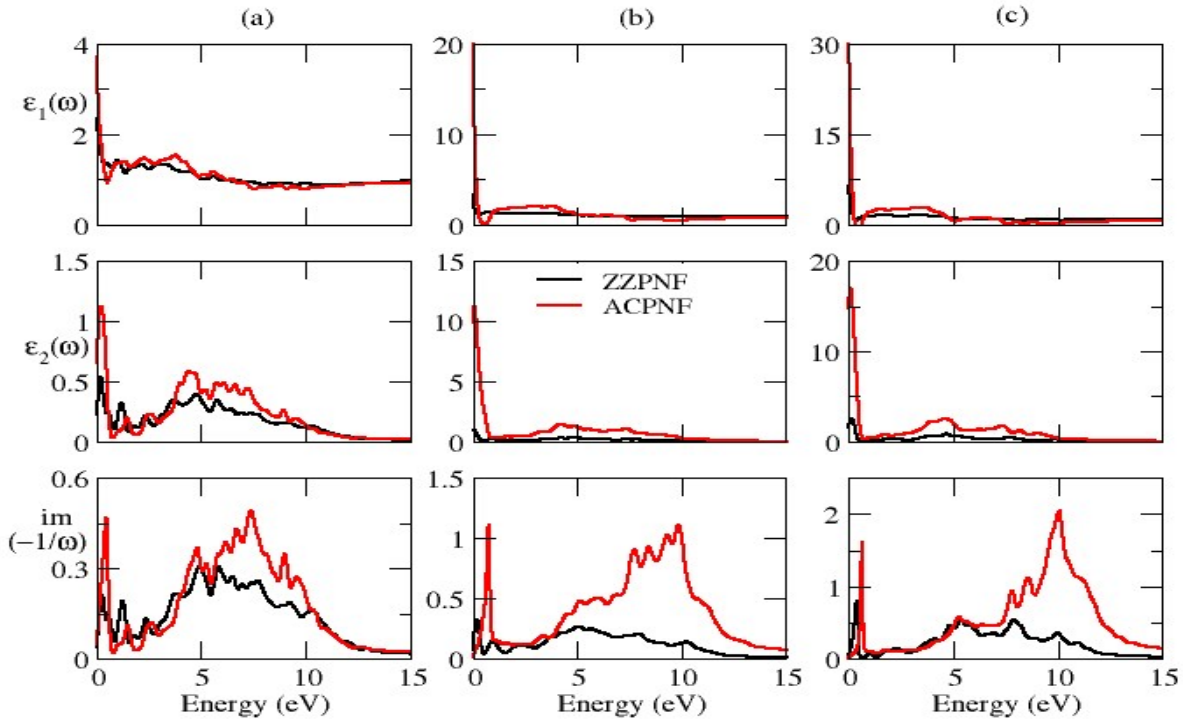

Figure S3: Real part of dielectric constant (ε_1), imaginary part of dielectric constant (ε_2), electron energy loss spectra of unpassivated ZZPNF and ACPNF with (a) triangular (T) (b) parallelogram (P) and (c) hexagonal (H) shape, for in-plan polarization.

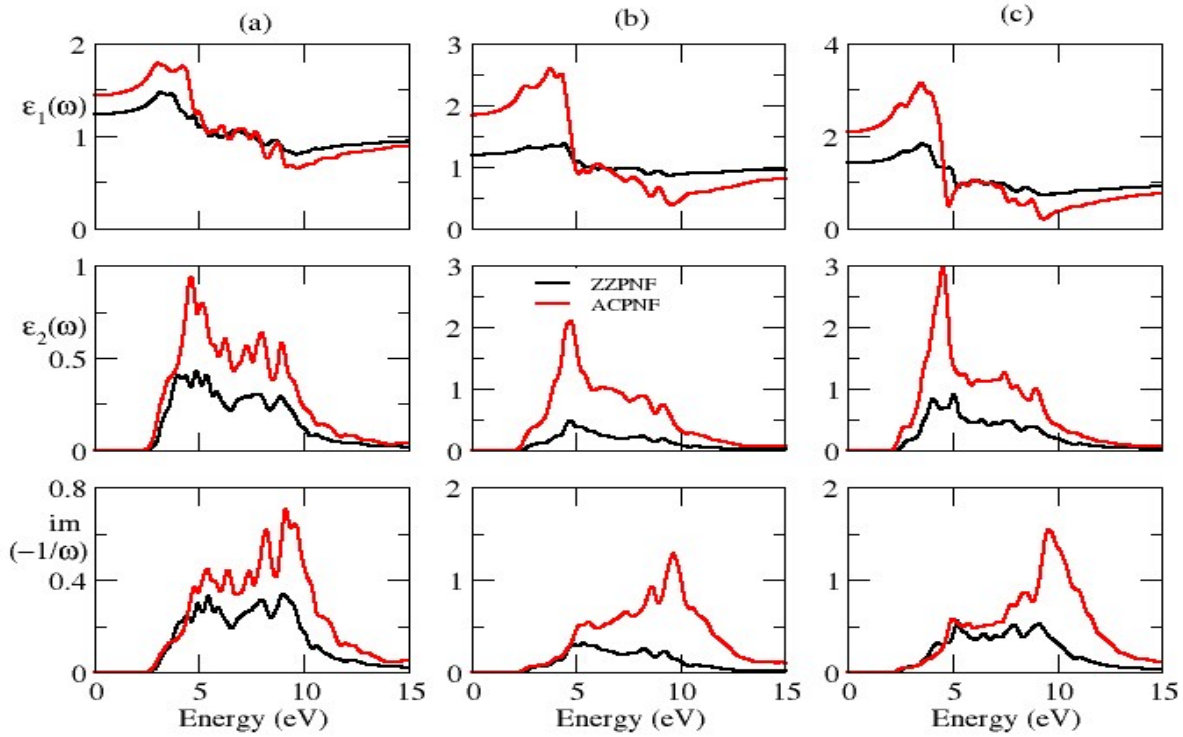

Figure S4: Real part of dielectric constant (ε_1), imaginary part of dielectric constant (ε_2), electron energy loss spectra of hydrogen passivated ZZPNF and ACPNF with (a) triangular (T) (b) parallelogram (P) and (c) hexagonal (H) shape, for in-plan polarization.

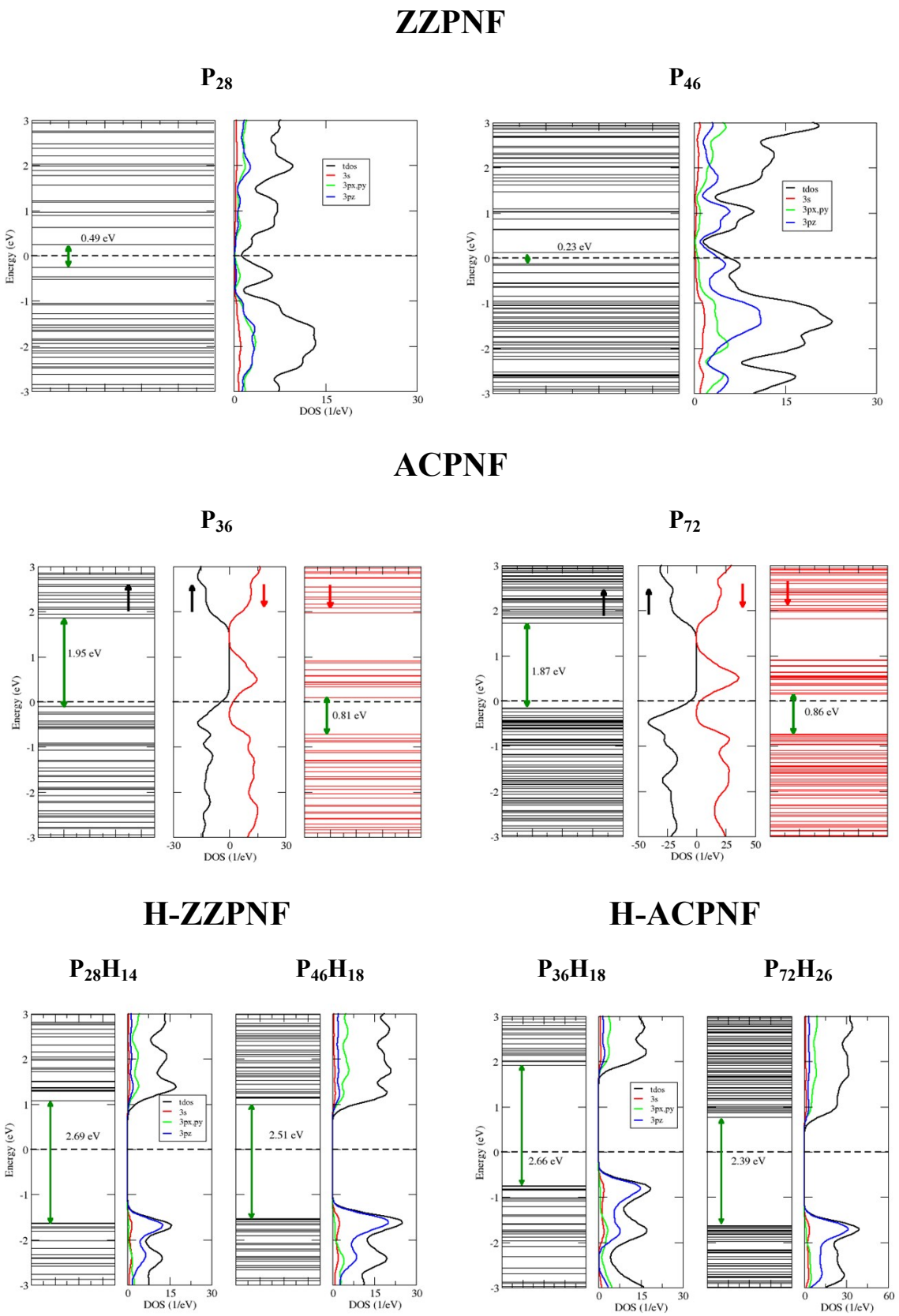

Figure S5: Parallelogram (P)-shaped zigzag (ZZ) and armchair (AC) nanoflakes with different number of P-atoms in bare and hydrogen-passivated PNFs.