Supporting Information:

Acute Mechano-Electronic Responses in Twisted Phosphorene Nanoribbons

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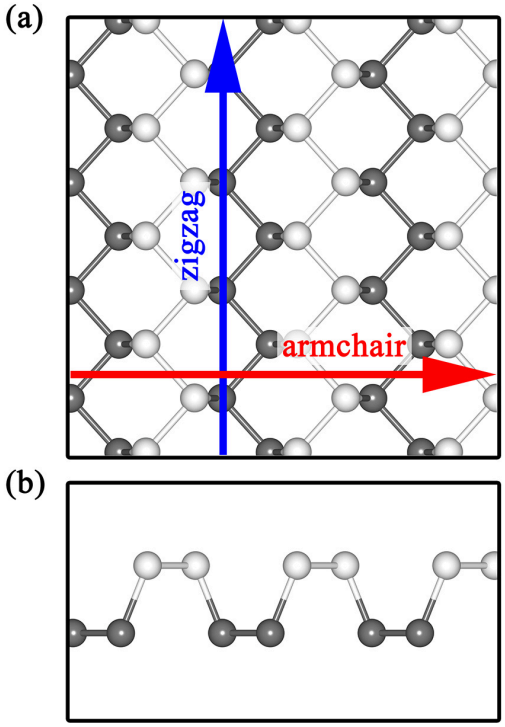

FIG. S1. (Color online) Top- and side-views of the atomic structure of pristine single-layered phosphorene in (a) and (b), respectively. Atoms with different vertical height are distinguished by the color of atoms. Armchair and zigzag direction is shown in red and blue arrow accordingly.

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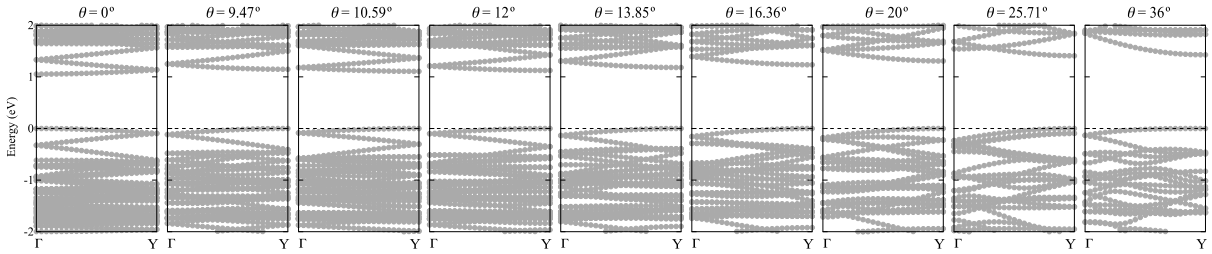


FIG. S2. (Color online) DFT-PBE electronic band structure of H-APNRs as a function of θ.

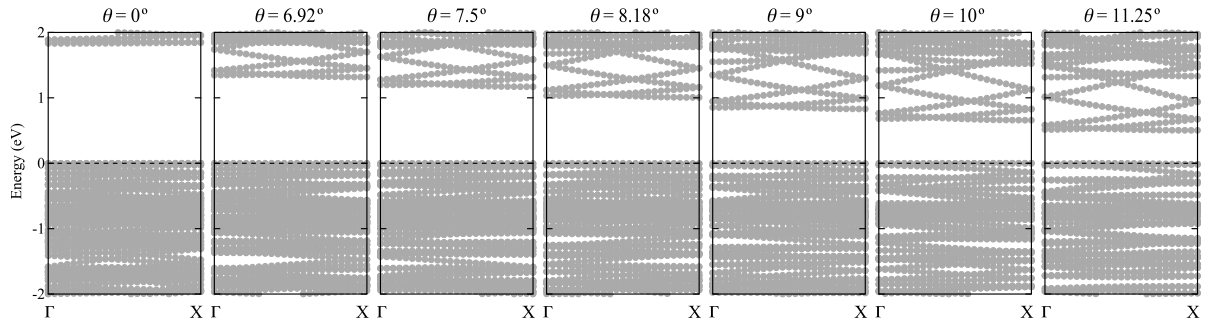


FIG. S3. (Color online) DFT-PBE electronic band structure of H-ZPNRs as a function of θ.

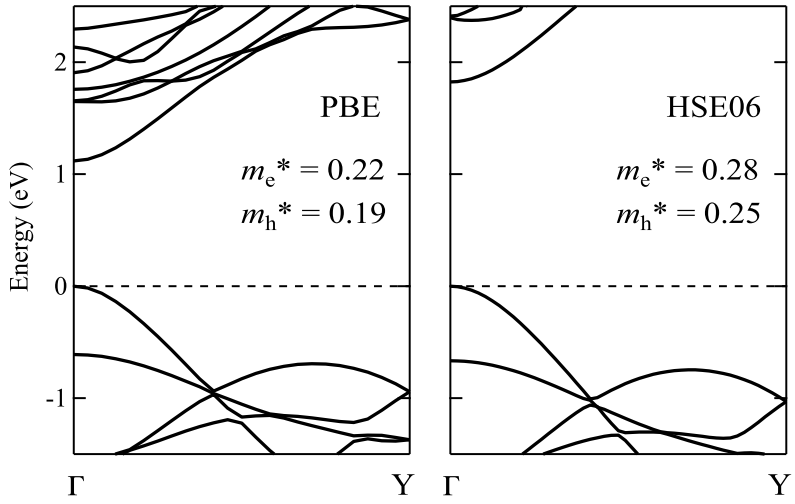


FIG. S4. (Color online) Comparison of the electronic band structure and its derived electron effective mass, m_e^* of untwisted H-APNR with (left) PBE and (right) HSE06 xc functional.

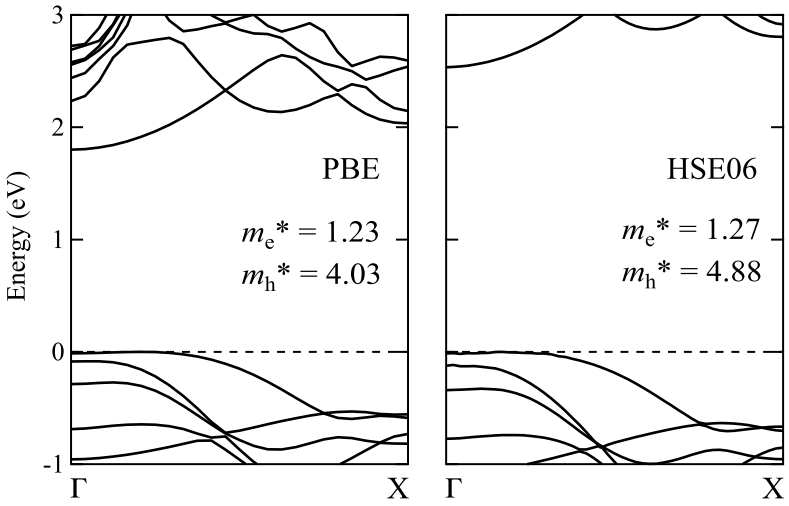


FIG. S5. (Color online) Comparison of the electronic band structure and its derived electron effective mass, m_e^* of untwisted H-ZPNR with (left) PBE and (right) HSE06 xc functional.

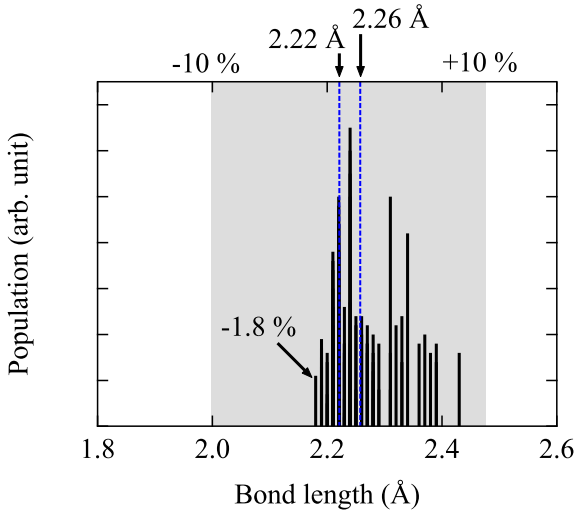
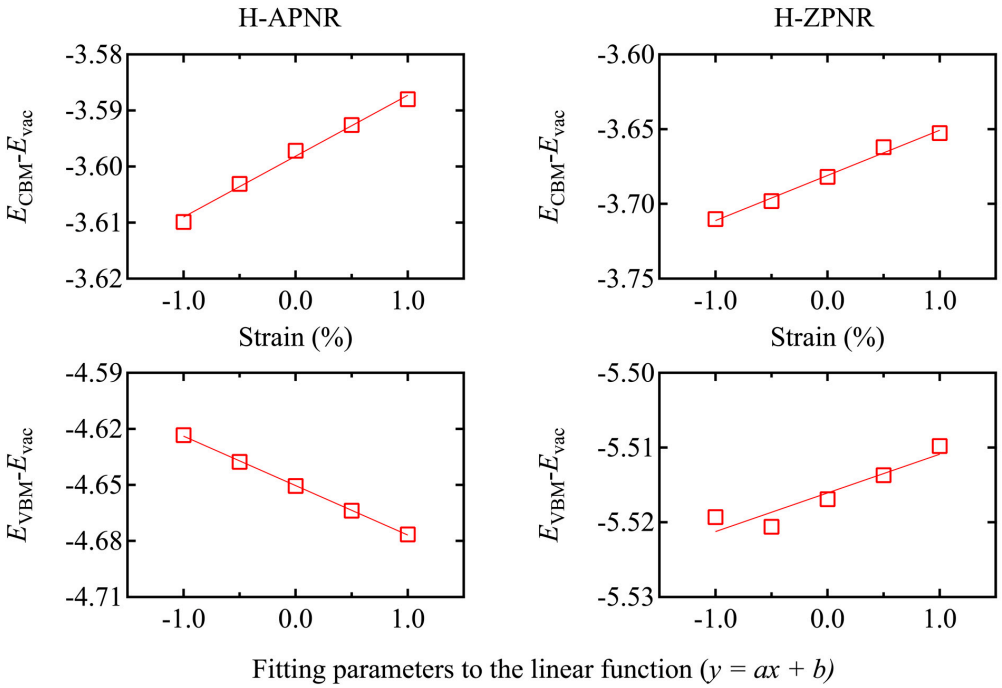


FIG. S6. (Color online) Population of P-to-P distances in H-APNRs and H-ZPNRs. ±10 % range is shown in grey shaded area. Optimized in-plane and out-of-plane P-P bond in unstrained phosphorene is shown in blue dotted lines.



Fitting parameters to the linear function ($y = ax + b$)

H-APNR	a	σ_a	b	σ_b	H-ZPNR	a	σ_a	b	σ_b
CBM	1.086	0.0571	-3.5982	0.000404	CBM	3.020	0.178	-3.6810	0.00126
VBM	-2.646	0.0321	-4.6504	0.000227	VBM	0.518	0.112	-5.5161	0.000795

FIG. S7. (Color online) Band energy of CBM and VBM in H-APNR (left) and H-ZPNR (right) with respect to the lattice dilation. HSE06 functional is used to calculate band energies. Fitting parameters (a and b) and standard deviations (σ_a and σ_b) are listed in the table.

TABLE S1. Computed effective masses and mobilities in H-APNRs. Parameters and constants used for the calculations are listed accordingly.

θ	θ/L	υ_0	C	E_1^{CBM}	E_1^{VBM}	m_e^*	m_h^*	μ_e	μ_h
degree	10^{-3}rad/Å	km s^{-1}	J m^{-2}	eV		m_0		10^3cm^{2}V^{-1}s^{-1}	
0	0	3.96	26.72	1.09	2.65	0.22	0.19	10.345	2.256
9.47	3.96	4.71	37.81	1.09	2.65	0.28	0.24	8.889	2.043
10.59	4.95	4.80	39.24	1.09	2.65	0.29	0.25	8.222	1.861
12.00	6.36	4.91	41.08	1.09	2.65	0.31	0.28	7.478	1.614
13.85	8.47	5.06	43.58	1.09	2.65	0.34	0.32	6.774	1.295
16.36	11.8	5.26	47.11	1.09	2.65	0.37	0.39	6.296	0.917
20.00	17.7	5.24	52.53	1.09	2.65	0.40	0.52	6.033	0.591
25.71	29.2	6.00	61.91	1.09	2.65	0.48	0.66	4.813	0.435
36.00	57.2	6.81	79.67	1.09	2.65	0.78	7.43	2.378	0.004

TABLE S2. Computed effective masses and mobilities in H-ZPNRs. Parameters and constants used for the calculations are listed accordingly.

θ	θ/L	v_0	C	E_1^{CBM}	E_1^{VBM}	m_e^*	m_h^*	μ_e	μ_h
degree	10^{-3}rad/Å	$\mathrm{km\,s^{-1}}$	$\mathrm{J\,m^{-2}}$	eV		m_0		$10^3\mathrm{cm^2V^{-1}s^{-1}}$	
0	0	7.99	90.27	3.02	0.52	1.23	4.03	0.139	0.438
6.92	2.80	7.91	89.36	3.02	0.52	0.20	6.37	5.306	0.173
7.50	3.29	7.90	89.57	3.02	0.52	0.22	5.23	4.430	0.257
8.18	3.91	7.89	89.83	3.02	0.52	0.25	5.00	3.495	0.283
9.00	4.73	7.88	90.22	3.02	0.52	0.31	5.72	2.242	0.217
10.00	5.84	7.87	91.04	3.02	0.52	0.44	63.98	1.110	0.002
11.25	7.39	7.86	92.33	3.02	0.52	0.87	0.65	0.282	17.053