

# Thermal/electric transmission properties regulation of armchair-phosphorene nanoscale devices based on defect engineering

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DV1			
Planar relationship	bonds type	number	Ave length(Å)
Different planes	P(H)–P(H)	2	2.2705
	P–P	6	2.2526
same plane	P(H)–P(H)	4	2.2636
	P–P	48	2.2498
	P–P(H)	12	2.2353
DV2			
Planar relationship	bonds type	number	Ave length(Å)
Different planes	P(H)–P(H)	1	2.2667
	P–P	7	2.1966
same plane	P(H)–P(H)	4	2.2646
	P–P	46	2.2423
	P–P(H)	14	2.2407
TDV1			
Planar relationship	bonds type	number	Ave length(Å)
Different planes	P(H)–P(H)	1	2.26
	P–P	7	2.2602
same plane	P(H)–P(H)	6	2.2603
	P–P	62	2.2432
	P–P(H)	18	2.2372
TDV2			
Planar relationship	bonds type	number	Ave length(Å)
Different planes	P(H)–P(H)	1	2.2647
	P–P	3	2.1782

same plane	P(H)–P(H)	2	2.2645
	P–P	24	2.2452
	P–P(H)	14	2.2442
TDV3			
Planar relationship	bonds type	number	Ave length(Å)
Different planes	P–P	7	2.2541
	P–P	-	-
same plane	P(H)–P(H)	4	2.2555
	P–P	42	2.2458
	P–P(H)	16	2.2409

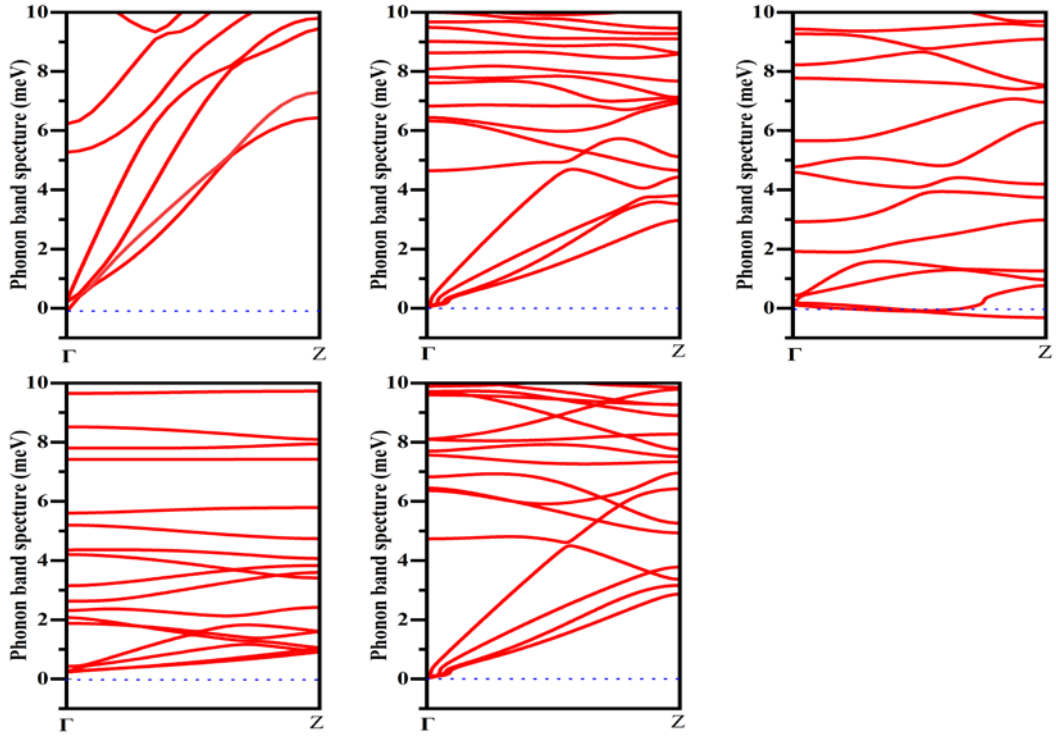
**Table S1** Statistical data of bond lengths for various types of different plane types.

DV1			
Planar relationship	angle type	number	Ave bond angle(°)
Different planes	H–P(H)	4	93.884
	P–P	20	101.952
	P–P(H)	8	102.635
same plane	H–P	12	92.925
	H–P(H)	8	93.478
	P–P	76	100.065
	P–P(H)	28	99.86

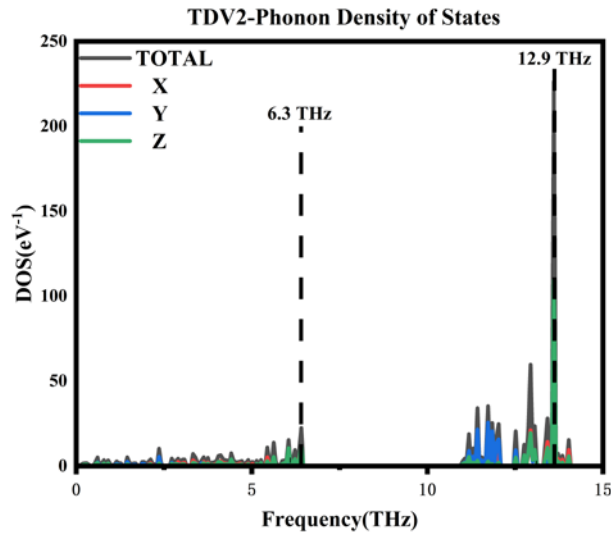
DV2			
Planar relationship	angle type	number	Ave bond angle (°)
Different planes	H-P(H)	2	93.487
	P-P	22	96.802
	P-P(H)	8	97.557
same plane	H-P	14	92.928
	H-P(H)	8	93.41
	P(H)-P(H)	2	103.229
	P-P	74	99.951
	P-P(H)	26	98.793
TDV1			
Planar relationship	angle type	number	Ave bond angle (°)
Different planes	H-P(H)	2	93.952
	P-P	22	102.875
	P-P(H)	8	103.289
same plane	H-P	18	92.355
	H-P(H)	12	93.789
	P(H)-P(H)	2	103.81
	P-P	102	100.437
	P-P(H)	38	100
TDV2			
Planar relationship	angle type	number	Ave bond angle (°)
Different planes	H-P(H)	2	92.834
	P-P	8	96.46
	P-P(H)	4	96.272
same plane	H-P	14	93.065

	H-P(H)	4	93.527
	P(H)-P(H)	4	103.139
	P-P	30	101.466
	P-P(H)	22	98.9
TDV3			
Planar relationship	angle type	number	Ave bond angle (°)
Different planes	P-P	20	101.333
	P-P(H)	8	103.038
same plane	H-P	16	91.927
	H-P(H)	8	93.829
	P(H)-P(H)	4	103.135
	P-P	70	99.717
	P-P(H)	24	99.414

**Table S2** Statistical data of bond lengths for various types of different plane types.



**Figure S1** Phonon band structure of APNRs with edge defects (a)APNRs, (b)DV2, (c)TDV1, (d)TDV2, (e)TDV3.



**Figure S2** The phonon density of states of TDV2, with two steep valleys and peaks corresponding to the phonon transmission spectrum at frequencies 6.3THz and 12.9THz respectively, are marked with vertical dashed lines.