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

all-phosphorus flexible device with non-collinear electrodes: A first principles study

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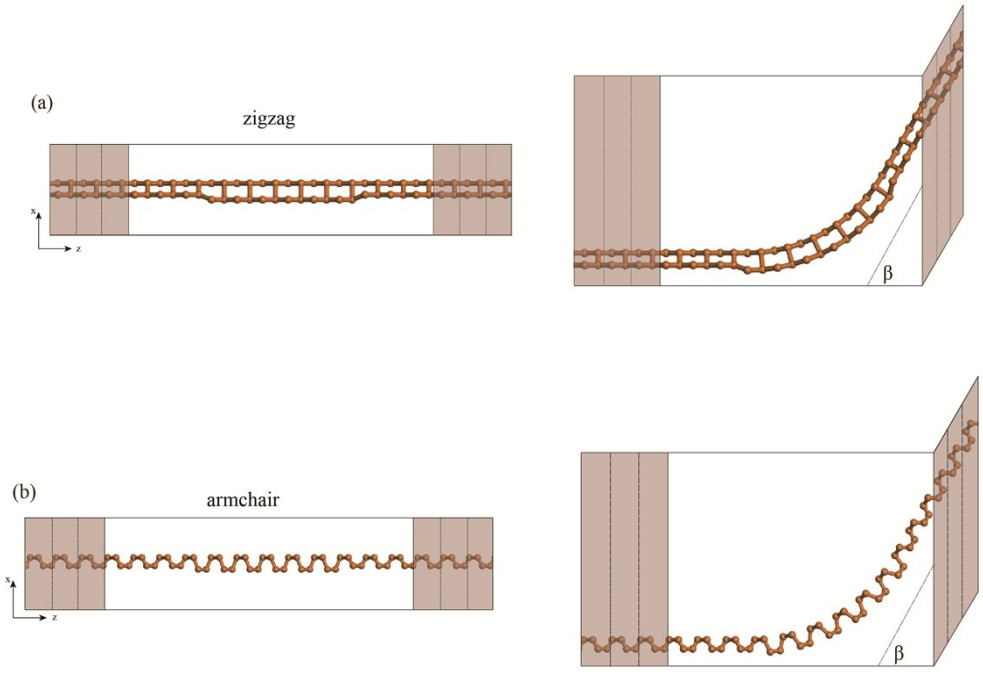
The side view of the atomic structures of the all-phosphorus devices. The transport is along the (a) zigzag and (b) armchair direction, respectively. The shadow regions indicate the electrodes which extend to the ±∞ along the transport direction. The angle between the two non-collinear electrodes is indicated by β. The non-orthogonal box allows the right electrode to extend along a non-collinear direction with respect to the left electrode.



Cartesian coordinates of the center scattering region of the zigzag all-phosphorus device with electrodes at β = 60° in this work.

	X(Å)	Y(Å)	Z(Å)
P	3.52779000	0.00000000	4.21214000
P	5.00000000	0.00000000	0.41285900
P	5.00000000	1.64900000	1.89964000
P	3.52779000	1.64900000	2.72536000
P	3.52779000	0.00000000	8.83714000
P	5.00000000	0.00000000	5.03786000
P	5.00000000	1.64900000	6.52464000
P	3.52779000	1.64900000	7.35036000
P	3.52779000	0.00000000	13.46210000
P	5.00000000	0.00000000	9.66286000
P	5.00000000	1.64900000	11.14960000
P	3.52779000	1.64900000	11.97540000
P	3.25742000	0.00000000	18.40230000
P	5.00322000	0.00000000	14.28780000
P	5.06806000	1.64900000	15.77300000
P	3.04798000	1.64900000	16.81150000
P	4.47263000	0.00000000	23.23770000
P	5.47744000	0.00000000	18.88260000
P	5.79920000	1.64900000	20.33390000
P	3.99013000	1.64900000	21.70740000
P	6.50905000	0.00000000	27.78860000
P	6.74233000	0.00000000	23.32510000
P	7.31122000	1.64900000	24.69860000
P	5.76814000	1.64900000	26.36530000
P	9.30477000	0.00000000	31.91670000
P	8.75944000	0.00000000	27.48060000
P	9.55818000	1.64900000	28.73430000
P	8.32797000	1.64900000	30.64370000
P	12.77490000	0.00000000	35.49670000
P	11.46750000	0.00000000	31.22260000
P	12.47180000	1.64900000	32.31860000
P	11.59190000	1.64900000	34.41260000
P	16.81390000	0.00000000	38.41960000
P	14.78420000	0.00000000	34.43750000
P	15.96360000	1.64900000	35.34250000
P	15.46060000	1.64900000	37.55750000
P	21.16140000	0.00000000	40.20510000
P	18.60720000	0.00000000	37.03050000
P	19.89480000	1.64900000	37.77390000
P	19.87380000	1.64900000	39.46170000

P	25.16670000	0.00000000	42.51760000
P	22.61260000	0.00000000	39.34300000
P	23.90020000	1.64900000	40.08640000
P	23.87910000	1.64900000	41.77420000
P	26.61790000	0.00000000	41.65550000
P	27.90550000	1.64900000	42.39890000

Cartesian coordinates of the center scattering region of the armchair all-phosphorus device with electrodes at β = 60° in this work.

	X(Å)	Y(Å)	Z(Å)
P	3.52779000	4.21214000	0.00000000
P	5.00000000	0.41285900	0.00000000
P	5.00000000	1.89964000	1.64900000
P	3.52779000	2.72536000	1.64900000
P	3.52779000	4.21214000	3.29800000
P	5.00000000	0.41285900	3.29800000
P	5.00000000	1.89964000	4.94700000
P	3.52779000	2.72536000	4.94700000
P	3.52779000	4.21214000	6.59600000
P	5.00000000	0.41285900	6.59600000
P	5.00000000	1.89964000	8.24500000
P	3.52779000	2.72536000	8.24500000
P	2.89684000	4.21214000	9.89400000
P	5.00000000	0.41285900	9.89400000
P	5.07191000	1.89964000	11.54090000
P	2.97675000	2.72536000	11.72420000
P	3.21587000	4.21214000	13.54050000
P	5.28707000	0.41285900	13.17530000
P	5.64387000	1.89964000	14.78470000
P	3.61237000	2.72536000	15.32900000
P	4.16325000	4.21214000	17.07620000
P	6.13958000	0.41285900	16.35690000
P	6.77042000	1.89964000	17.87990000
P	4.86431000	2.72536000	18.76870000
P	5.71021000	4.21214000	20.39370000
P	7.53160000	0.41285900	19.34210000
P	8.41733000	1.89964000	20.73240000
P	6.69452000	2.72536000	21.93870000
P	7.80975000	4.21214000	23.39210000
P	9.42086000	0.41285900	22.04020000
P	10.53460000	1.89964000	23.25560000
P	9.04740000	2.72536000	24.74280000

P	10.39810000	4.21214000	25.98040000
P	11.74990000	0.41285900	24.36930000
P	13.05780000	1.89964000	25.37280000
P	11.85140000	2.72536000	27.09560000
P	13.71200000	4.21214000	27.53350000
P	14.44810000	0.41285900	26.25850000
P	15.87610000	1.89964000	27.08300000
P	15.14000000	2.72536000	28.35800000
P	16.56810000	4.21214000	29.18250000
P	17.30420000	0.41285900	27.90750000
P	18.73230000	1.89964000	28.73200000
P	17.99620000	2.72536000	30.00700000
P	19.42430000	4.21214000	30.83150000
P	20.16040000	0.41285900	29.55650000
P	21.58850000	1.89964000	30.38100000