

Supporting Information

High Mobility in α -Phosphorene Isostructures with the Low Deformation Potential

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S1 Anisotropic effective mass of two carriers in all structures

Table S1. Anisotropic effective mass (m_{ij}) of both hole (h) and electrons (e) of α -phosphorene isostructures, unit (m_e)

isostructures	hole mass in the zigzag direction (m_{hx})	hole mass in the armchair direction (m_{hy})	electron mass in the zigzag direction (m_{ex})	electron mass in the armchair direction (m_{ey})
α -phosphorene	4.99	0.15	1.24	0.17
α - arsenene	1.45	0.21	1.16	0.35
α -graphane	0.29	0.96	1.03	0.84
α -silicane	0.22	1.21	0.15	3.77
α -PAs	1.67	0.20	1.16	0.23
α -PCH	9.03	0.39	0.58	0.80
α -PSiH	9.19	0.48	0.20	1.34
α -AsCH	7.52	0.44	0.60	0.91
α -AsSiH	6.03	0.48	0.17	1.01
α -CHSiH	0.32	1.30	0.80	1.15

S2 The specific values of carrier mobility of both carriers in all structures

Table S2. Anisotropic carrier mobility (μ_{ij}) of both hole (h) and electrons (e) of α -phosphorene isostructures, unit ($\text{cm}^2\text{V}^{-1}\text{s}^{-1}$)

isostructures	μ_{hx}	μ_{hy}	μ_{ex}	μ_{ey}
α -phosphorene	2.70×10^4	8.91×10^2	9.23×10^1	1.60×10^3
α - arsenene	3.01×10^2	6.11×10^1	1.19×10^2	1.12×10^2
α -graphane	1.77×10^2	6.37×10^1	3.67×10^3	4.60×10^5
α -silicane	7.74×10^2	3.60×10^2	2.94×10^2	4.82
α -PAs	9.14×10^1	3.50×10^2	1.05×10^2	1.96×10^4
α -PCH	1.26×10^1	1.52×10^1	4.31×10^2	8.81×10^3
α -PSiH	7.77×10^1	1.43×10^1	2.61×10^2	1.64×10^1
α -AsCH	1.36×10^1	2.03×10^1	9.88×10^2	1.14×10^4
α -AsSiH	1.71×10^2	1.41×10^2	5.59×10^2	3.99×10^1
α -CHSiH	2.35×10^2	1.63×10^1	8.64×10^2	3.37×10^1

S3 The calculation details of carrier mobility and its key parameters of β -graphane

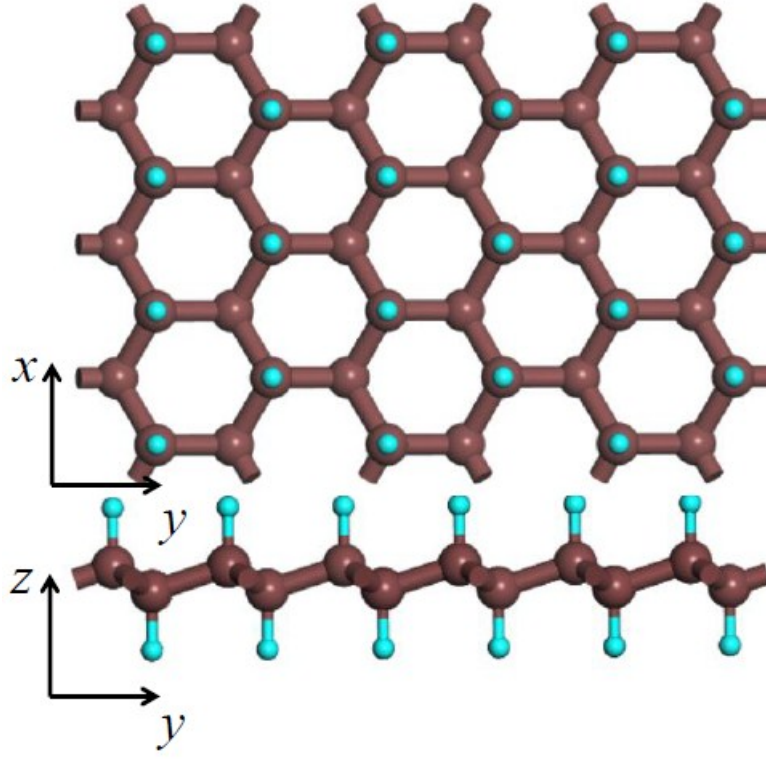


Figure S1 The anisotropic geometry structure of β -graphane. x represents the zigzag direction while y represents the armchair direction.

Table S3. The calculation details of β -graphane

directions	carrier type	lattice constant (Å)	m	E	C_{2D}	μ
The zigzag (x)	hole	2.51	0.60	1.52	0.95	6.08×10^2
	electron		0.25	6.04		5.68×10^1
The armchair (y)	hole	4.34	1.01	0.72	0.59	6.24×10^2
	electron		0.98	0.82		3.11×10^2

The β -graphane has the similar structure to β -phosphorene (the blue phosphorus). The comparison of values of carrier mobility between β -graphane to α -graphane is similar to that between β -phosphorene and α -phosphorene. The carrier mobility of β -graphane is quite small compared to α -graphane. And these results are in agreement with the experimental measurement¹⁻³.

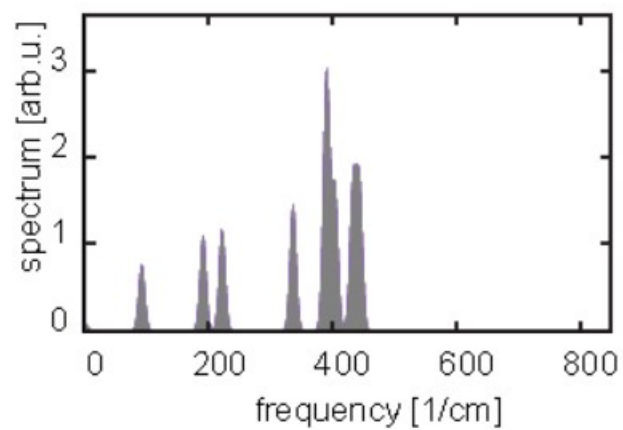
S4 Elastic Modulus of these structures**Table S4** Calculated elastic Moduli (unit: kBar) for various structures based on DFT-GGA.

isostructures	C_{11}	C_{12}	C_{22}	C_{13}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
α -arsenene	114.35	63.29	187.34	190.49	48.56	250.26	18.88	48.22	163.28
α -graphane	1104.8	194.43	1268.5	302.43	227.36	1500.4	387.89	651.38	664.86
α -silicane	341.50	24.93	375.50	141.51	134.46	375.32	54.46	219.05	181.64
α -PAs	183.82	118.76	290.55	267.97	90.61	508.12	60.11	103.26	297.57
α -PCH	641.05	119.08	744.41	252.47	132.41	1063.5	251.98	427.17	471.14
α -PSiH	336.11	41.77	373.55	169.27	81.92	415.30	66.96	187.87	226.27
α -AsCH	285.15	57.54	428.20	185.88	88.70	562.48	124.89	247.53	242.26
α -AsSiH	297.30	31.79	348.10	173.44	72.10	402.51	58.77	1732.9	209.98
α -CHSiH	621.99	57.50	689.03	199.13	223.99	679.69	146.39	409.05	345.79

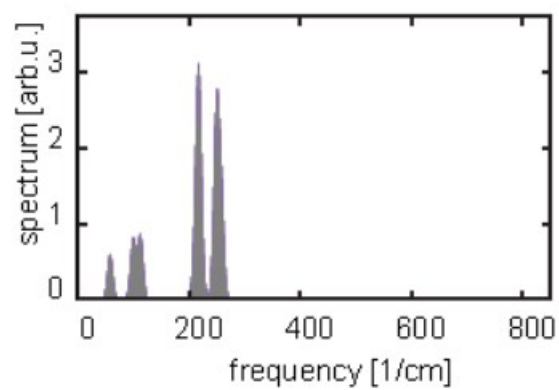
S5 Calculated vibrational frequency diagrams for various structures based on DFT-GGA

Figure S2 phonon vibration diagram

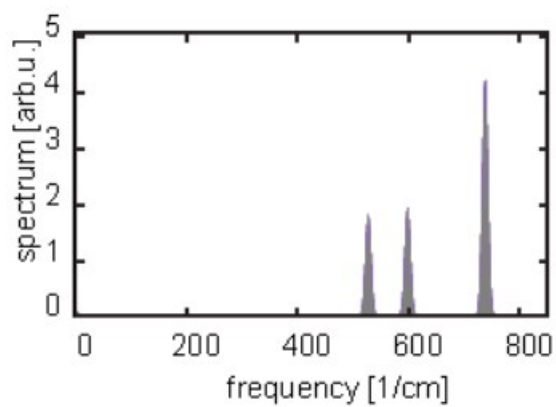
(a) phosphorene



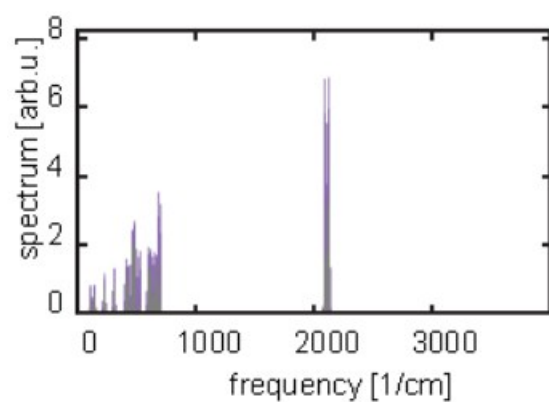
(b) arsenene



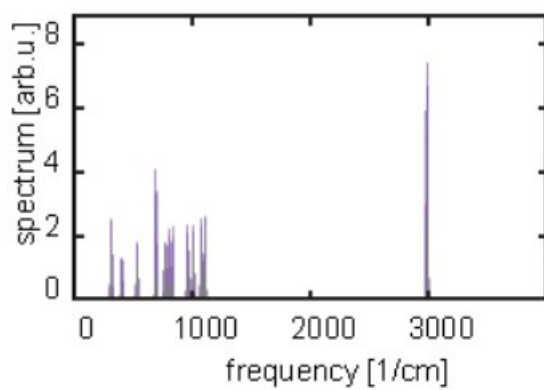
(c) graphane



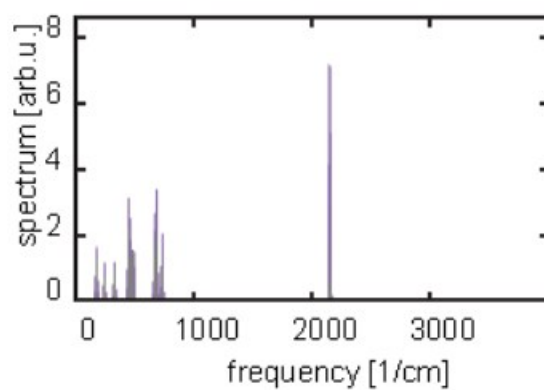
(d)silicene



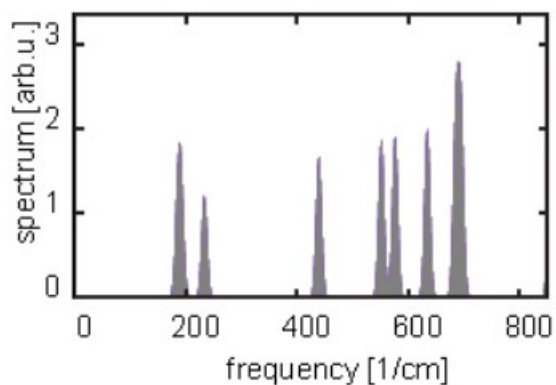
(e)P-CH



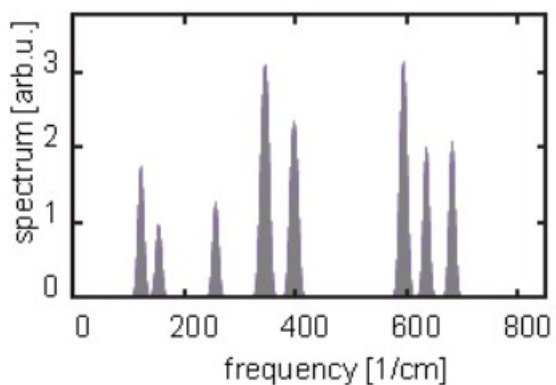
(f)P-SiH



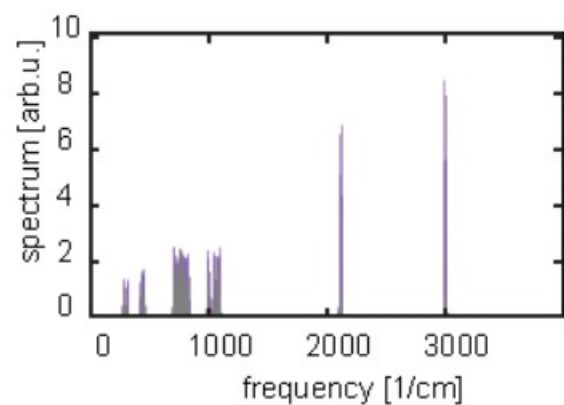
(g)As-CH



(h)As-SiH



(i)CH-SiH



References

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2. Jiang, S.; Arguilla, M. Q.; Cultrara, N. D.; Goldberger, J. E. Covalently-controlled properties by design in group IV graphane analogues. *Accounts of Chemical Research* **2014**, 48 (1), 144-151.

3. Elias, D. C.; Nair, R. R.; Mohiuddin, T.; Morozov, S.; Blake, P.; Halsall, M.; Ferrari, A.; Boukhvalov, D.; Katsnelson, M.; Geim, A. Control of graphene's properties by reversible hydrogenation: evidence for graphane. *Science* **2009**, 323 (5914), 610-613.