Supplementary Information

Orthorhombic Si_6: Prediction of a metastable sp^3 silicon semimetal with pseudo-Dirac nodal line

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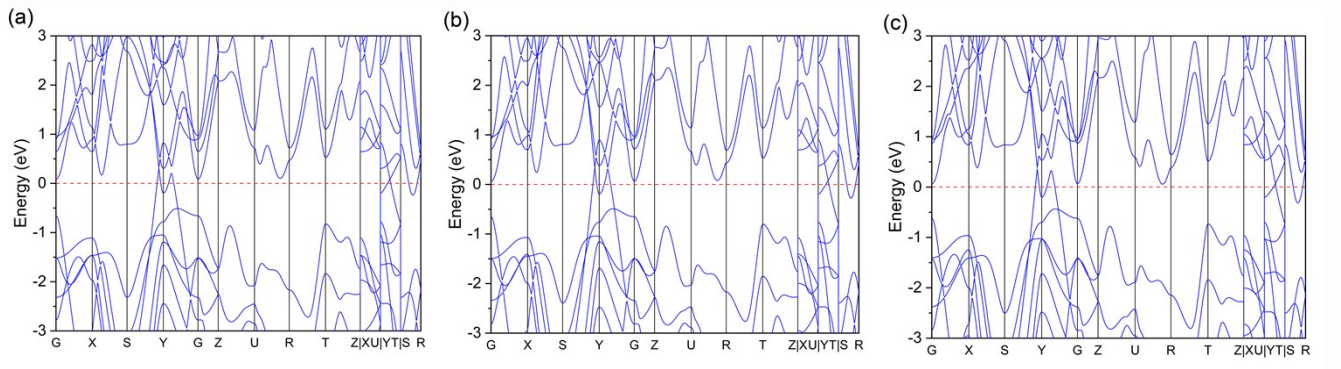

Fig. S1 Band structures of oP-Si_6 calculated by DFT-PBE at (a) 3 GPa, (b) 6 GPa, (c) 12 GPa in hydrostatic condition.

Table S1 The calculated elastic constants C_{ij}, bulk moduli B (GPa), and shear moduli G (GPa) of fully-relaxed oP-Si_6 and Si-I phase at 0 GPa by PBE functional.

Phase	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{23}	B	G
Si-I	153			99			57			89	74
oP-Si_6	201	175	234	110	75	103	61	21	38	95	88

Table S2 Calculated *d*-spacings (Å, d_{cal}) of oP-Si_6 (fully-relaxed by both LDA and GGA functional at 0 GPa) compared with the experimental *d*-spacings (Å, d_{obs}) from both synchrotron XRD reflections and FFT electron diffractions in Ref.30. Quenstion marks indicate the measured *d*-spacings from unknown structures. $(d_{obs.}-d_{cal.})/d_{obs.}(\%)$ represent the *d*-spacing error between the XRD and the simulated value.

oP-Si_6	LDA		GGA			XRD	FFT
（hkl）	d_{cal} (Å)	$(d_{obs.}-d_{cal.})/d_{obs.}(\%)$	d_{cal} (Å)	$(d_{obs.}-d_{cal.})/d_{obs.}(\%)$	I/Imax	$d_{obs}\pm\Delta d$ (Å)	$d_{obs}\pm\Delta d$ (Å)
(001)	6.863		6.944		0		
（010）	3.985		4.042		0.2		4.2±0.23
(100)	3.822		3.871		27.0		3.82±0.20
(011)	3.446		3.493		0		3.60±0.17 (??)
(002)	3.432		3.472		19.2		
(101)	3.339		3.381		0		3.29±0.14
(110)	2.758	0.6	2.796	-0.8	19.7	2.774±0.009 (?)	2.73±0.10
		0.2		-1.1		2.765±0.008 (?)	
(012)	2.600	1.7	2.634	0.45	60.7	2.646±0.007 (??)	2.64±0.09
		0.6		-0.3		2.616±0.007	
(111)	2.559		2.593		100		
(102)	2.553	-3.9E-4	2.585	-1.3	15.1	2.552±0.007 (?)	2.51±0.08
(003)	2.288		2.314		0		2.29±0.07
(112)	2.150	1.6	2.177	0.4	18.2	2.185±0.005	2.21±0.06
(020)	1.992		2.021		0.1		2.00±0.05
(013)	1.984		2.008		0		
(103)	1.963		1.986		0		
(021)	1.913	0.4	1.940	-1.0	0	1.920±0.005	
(200)	1.911	-0.3	1.936	-1.6	3.0	1.906±0.005	1.91±0.05
(201)	1.841		1.864		0		1.82±0.04
(120)	1.767		1.792		4.5		1.77±0.04
(113)	1.761		1.783		28.4		
(022)	1.723		1.747		19.6		
(210)	1.723		1.746		15.2		
(004)	1.716		1.736		18.4		1.71±0.04
(121)	1.711		1.735		21.5		
(211)	1.671		1.693		0.01		
(202)	1.669	0.6	1.690	-0.6	**33.3**	1.679±0.004 (?)	
(014)	1.576		1.595		0.02		
(122)	1.571		1.592		6.1		
(104)	1.565		1.584		3.0		
(212)	1.540		1.560		0.04		1.55±0.03
(023)	1.502		1.522		0		
(203)	1.466		1.485		0		1.49±0.03
(114)	1.457		1.475		4.4		
(123)	1.398	0.1	1.417	-1.2	10.1	1.400±0.003	1.42±0.03
(220)	1.379		1.398		8.5		
(213)	1.376		1.394		0.03		
(005)	1.373		1.389		0		
(221)	1.352		1.370		0.03		1.36±0.02
(030)	1.328	1.5	1.347	7.4E-4	7.0	1.348±0.003 (??)	
(031)	1.304		1.323		0		1.31±0.02
(024)	1.300		1.317		0.04		
(015)	1.298		1.313		0		
(105)	1.292		1.307		0		

oP-Si_6	LDA		GGA			XRD	FFT
（hkl）	d_{cal} (Å)	$(d_{obs.}-d_{cal.})/d_{obs.}$(%)	d_{cal} (Å)	$(d_{obs.}-d_{cal.})/d_{obs.}$(%)	I/Imax	$d_{obs}\pm\Delta d$ (Å)	$d_{obs}\pm\Delta d$ (Å)
(222)	1.280		1.297		0.1		
(204)	1.277		1.292		1.3		
(300)	1.274		1.290		0.6		
(130)	1.255		1.272		1.3		
（301）	1.252		1.269		0		
(032)	1.239	0.24	1.256	-1.1	1.2	1.242±0.002	
(131)	1.234		1.252		0.2		
(124)	1.231		1.247		1.1		1.23±0.02
(115)	1.229		1.244		7.3		
(214)	1.216		1.231		8.1		
(310)	1.213	0	1.229	-1.3	1.2	1.213±0.002	
(311)	1.195	0.9	1.210	-0.3	6.6	1.206±0.002 (??)	1.20±0.02
(302)	1.194	0.5	1.209	-0.8	1.2	1.200±0.002 (??)	
(223)	1.181		1.196		1.6E-3		
(132)	1.178		1.195		1.9		
(033)	1.149		1.164		0		
(312)	1.144		1.159		1.7		
(006)	1.144		1.157		0.4		
(025)	1.130		1.144		0		
(205)	1.115		1.128		0		
(303)	1.113		1.127		0		
(133)	1.100		1.115		0.1		
(016)	1.099	0.6	1.112	-0.5	2.8	1.106±0.002	1.10±0.02
(106)	1.096		1.109		0.7		
(230)	1.091		1.106		0.7		
(125)	1.084		1.098		3.9		
(231)	1.077		1.092		3.7E-5		
(224)	1.075		1.089		6.8		
(320)	1.073		1.088		0.8		
(215)	1.074		1.087		1.3E-3		
(313)	1.072		1.086		4.5		
(321)	1.060		1.074		3.7		1.07±0.01 (??)
(116)	1.056		1.069		0.7		
(034)	1.050		1.064		6.0		
(232)	1.039	0.8	1.054	-0.7	11.6	1.047±0.002	1.04±0.01
(322)	1.024		1.038		1.2		
(304)	1.023		1.036		0.3		
(134)	1.013		1.026		1.3		
(040)	0.996		1.010		3.8E-2		
(026)	0.992		1.004		2.7		
(314)	0.991		1.003		1.2		
(041)	0.986		1.000		0		
(233)	0.984		0.998		2.9E-5		
(206)	0.981		0.993		5.1		
(007)	0.980		0.992		0		
(225)	0.973		0.985		8.6E-4		
(323)	0.972		0.984		2.9		
(140)	0.964		0.978		0.5		
(126)	0.960		0.972		1.1		
(042)	0.957	0.2	0.970	-1.1	1.4	0.959±0.002	