Supporting information for

Si_3AlP: a new promising material for solar cell absorber

Ji-Hui Yang[†], Yingteng Zhai[†], Hengrui Liu[†], Hongjun Xiang[†*], Xingao Gong[†*], and Su-Huai Wei[‡]

[†] *Key Laboratory of Computational Physical Sciences (Ministry of Education), State Key Laboratory of Surface Physics, and Department of Physics, Fudan University, Shanghai 200433, P. R. China*

[‡] *National Renewable Energy Laboratory, Golden, Colorado 80401, USA*

I. Lattice vectors and atomic positions of the *Cc*-Si_3AlP phase

The unrelaxed lattice vectors of primitive cell for *Cc*- Si_3AlP are

a_1 = (1.00 -0.50 0.50)

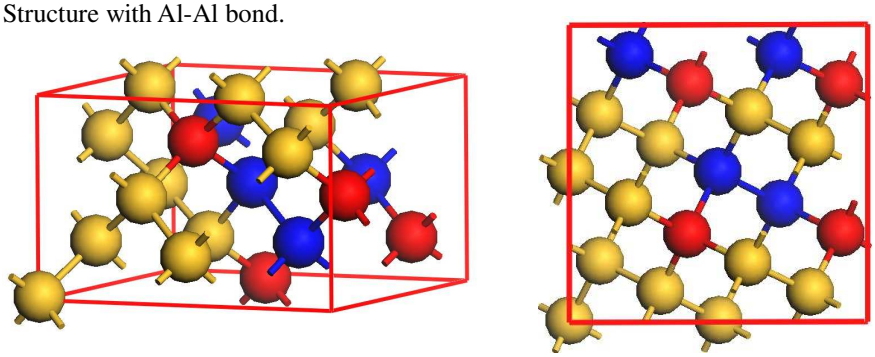
a_2 = (1.00 0.50 0.50)

a_3 = (-1.50 0.00 0.50)

The unrelaxed atomic positions within the unit cell (in direct lattice coordinates) are

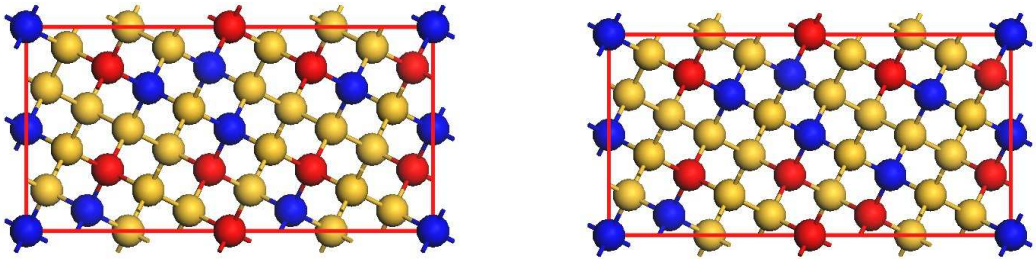
Si	0.00	0.00	0.00
Si	0.40	0.40	0.20
Si	0.55	0.05	0.90
Si	0.75	0.25	0.50
Si	0.15	0.65	0.70
Si	0.80	0.80	0.40
Al	0.95	0.45	0.10
Al	0.20	0.20	0.60
P	0.60	0.60	0.80
P	0.35	0.85	0.30

II. Structure with Al-Al bond.



The red balls are P, blue balls are Al and yellow balls are Si. We find that formation of Al-Al bond is strongly energetically unfavorable.

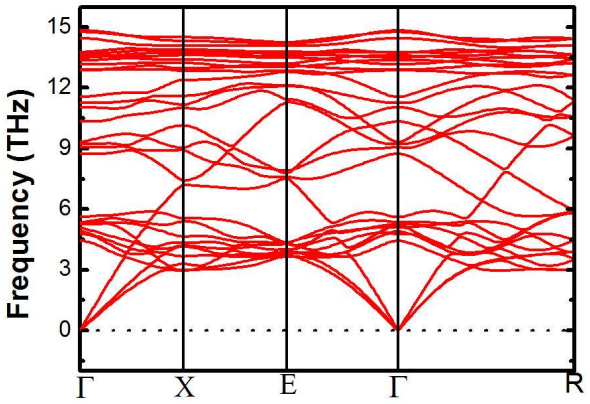
III. Si_3AlP with 40-atoms structures for the test



Structure 1 Structure 2

This figure shows two 40-atoms structures randomly generated for our tests. The first one has an energy of 25 meV/atom higher than the *Cc* structure and the second one has an energy of 42 meV/atom higher.

IV. Phonon spectrum of *Cc*-Si_3AlP



We calculated the phonon spectrum of *Cc*-Si_3AlP using PHONOPY package. As we can see, there are no imaginary phonon modes, suggesting the dynamic stability of this structure.

V. Bader analysis of charge on each atomic sites for *Cc*-Si_3AlP

Through the Bader analysis, we find that for *Cc*-Si_3AlP the net charge on Si site is about -0.09, the net charge state on Al site is about 1.72, and the net charge on P site is about -1.45.

VI. LDA calculated lattice parameters of Si_3AlP, Si, and AlP in the 20-atoms cell:

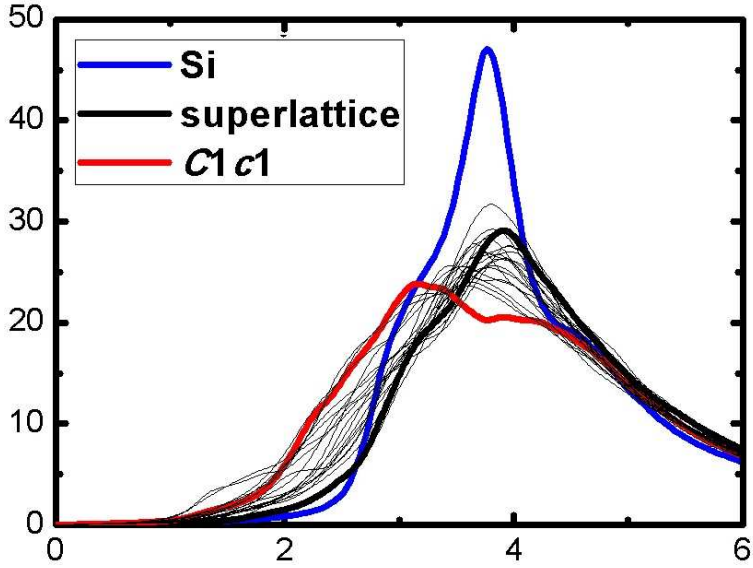
structure	**a**	**b**	**c**	**α**	**β**	**γ**	**Lattice mismatch to Si**
Si	8.5422	8.5422	5.4026	90	90	90	0
AlP	8.5864	8.5864	5.4351	90	90	90	0.52%
Cc-Si_3AlP	8.5505	8.5806	5.4642	90	90	89.6606	0.45%
$P1_1$-Si_3AlP	8.5706	8.5705	5.4524	90.0000	90.0000	90.0000	0.33%
$P1_2$-Si_3AlP	8.5699	8.5699	5.4519	90.0003	89.9999	90.0000	0.32%
$P1_3$-Si_3AlP	8.5521	8.5810	5.4622	89.9815	90.1029	90.0978	0.45%
$P1_4$-Si_3AlP	8.5650	8.5555	5.4724	90.0001	90.0000	90.2449	0.27%
$P1_5$-Si_3AlP	8.5621	8.5928	5.4494	90.0001	90.0001	90.3840	0.59%

Since the Si_3AlP cell is grown on the Si (001) surface, we only considered **a** vector and **b** vector to calculate the lattice mismatch between Si_3AlP and Si. The larger one of **a** and **b** (we use **a** in the following formula) is used and the lattice mismatch is calculated according to:

$$\text{Lattice mismatch}=(\mathbf{a}_{\mathbf{Si3AlP}}-\mathbf{a}_{\mathbf{Si}})/\mathbf{a}_{\mathbf{Si}}$$

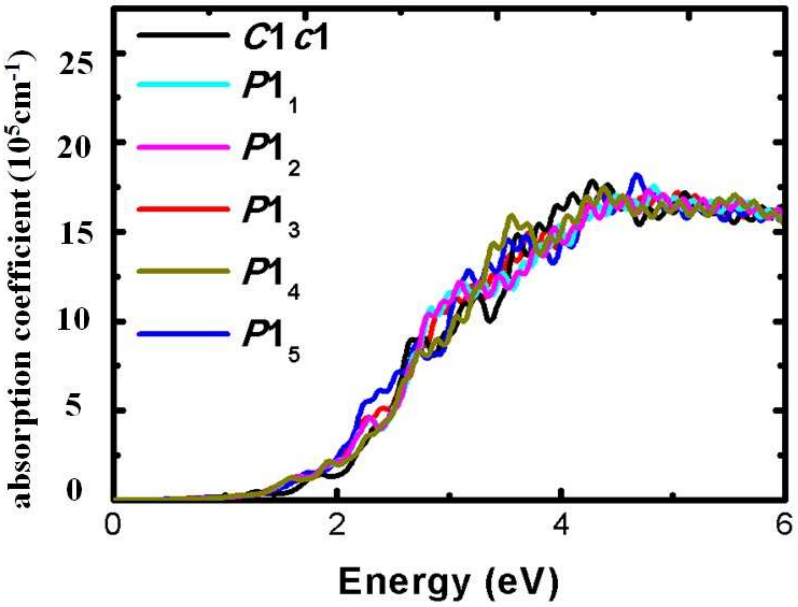
As we can see, the lattice mismatch between Si_3AlP and Si is very small and almost negligible. Besides, the lattice is only a little distorted and can be neglected.

VII. Calculated imaginary dielectric function of the 10-atom structures that are more energetically stable than the *Cc*-structure.



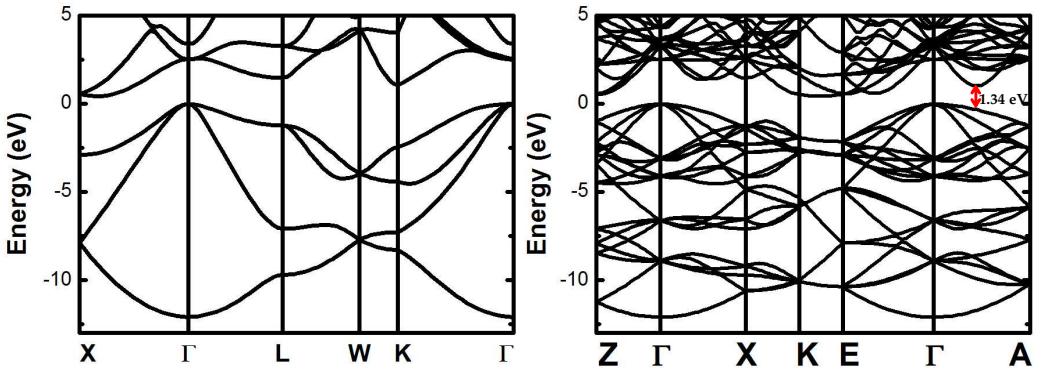
The LDA calculated optical spectrum of these structures show that they generally have their values in between the superlattice structure and *Cc*-structure. Some of them also show metallic behavior, which is not plotted here. We find that *Cc*-structure gives the best optical properties for solar cell applications.

VIII. Absorption coefficients of other structure with [$AlPSi_3$] arrangements.



As we can see, the absorption spectrums are almost the same for all the six structures. This indicates that the optical properties of these materials are not sensitive to the atomic arrangements in the unit cell once the local structural motif is preserved, which provides convenience for the synthesis.

IX. band structures of Si in its 2-atoms primitive cell and 10-atoms *Cc* cell



Si_2 Si_{10}

In the Si 2-atoms primitive cell, the LDA calculated minimum direct band gap is at Γ point and has a value of 2.53 eV; in the Si 10-atoms *Cc* cell, the minimum pseudo direct band gap appears to be at a point along Γ-A line and has a value of 1.34 eV, as shown in the figure. But the transition at this point is not allowed in pure Si, because the CBM state and VBM state are folded from two different k-points of the original 2-atom Si cell. After AlP is mixed, the transition becomes allowed due to the reduction of the symmetry.

X. Electron characters at the special k-points in the same 10-atoms cell for Si and *Cc*-Si_3AlP. Si_{10} cell

Special k-points	Z					G					X					K				
VB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.000	0.073	0.000	0.073	1	0.000	0.044	0.000	0.044	1	0.000	0.045	0.000	0.045	1	0.000	0.033	0.000	0.033
	2	0.002	0.044	0.000	0.046	2	0.000	0.044	0.000	0.044	2	0.000	0.045	0.000	0.045	2	0.001	0.056	0.000	0.056
	3	0.001	0.059	0.000	0.060	3	0.000	0.044	0.000	0.044	3	0.000	0.045	0.000	0.045	3	0.001	0.067	0.000	0.068
	4	0.004	0.012	0.000	0.015	4	0.000	0.044	0.000	0.044	4	0.000	0.045	0.000	0.045	4	0.000	0.021	0.000	0.021
	5	0.003	0.021	0.000	0.024	5	0.000	0.044	0.000	0.044	5	0.000	0.045	0.000	0.045	5	0.000	0.026	0.000	0.027
	6	0.004	0.010	0.000	0.014	6	0.000	0.044	0.000	0.044	6	0.000	0.045	0.000	0.045	6	0.000	0.034	0.000	0.034
	7	0.002	0.039	0.000	0.041	7	0.000	0.044	0.000	0.044	7	0.000	0.045	0.000	0.045	7	0.000	0.045	0.000	0.046
	8	0.003	0.024	0.000	0.028	8	0.000	0.044	0.000	0.044	8	0.000	0.045	0.000	0.045	8	0.001	0.072	0.000	0.073
	9	0.000	0.071	0.000	0.072	9	0.000	0.044	0.000	0.044	9	0.000	0.045	0.000	0.045	9	0.000	0.029	0.000	0.030
	10	0.001	0.062	0.000	0.063	10	0.000	0.044	0.000	0.044	10	0.000	0.045	0.000	0.045	10	0.000	0.022	0.000	0.023
	tot	0.020	0.415	0.000	0.436	tot	0.000	0.441	0.000	0.441	tot	0.000	0.446	0.000	0.446	tot	0.004	0.407	0.000	0.411
CB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.013	0.005	0.000	0.018	1	0.000	0.031	0.000	0.031	1	0.038	0.004	0.000	0.041	1	0.011	0.011	0.000	0.021
	2	0.013	0.005	0.000	0.018	2	0.000	0.031	0.000	0.031	2	0.038	0.004	0.000	0.041	2	0.011	0.011	0.000	0.021
	3	0.013	0.005	0.000	0.018	3	0.000	0.031	0.000	0.031	3	0.038	0.004	0.000	0.041	3	0.011	0.011	0.000	0.021
	4	0.013	0.005	0.000	0.018	4	0.000	0.031	0.000	0.031	4	0.038	0.004	0.000	0.041	4	0.011	0.011	0.000	0.021
	5	0.013	0.005	0.000	0.018	5	0.000	0.031	0.000	0.031	5	0.038	0.004	0.000	0.041	5	0.011	0.011	0.000	0.021
	6	0.008	0.008	0.000	0.017	6	0.000	0.031	0.000	0.031	6	0.038	0.004	0.000	0.041	6	0.011	0.011	0.000	0.021
	7	0.008	0.008	0.000	0.017	7	0.000	0.031	0.000	0.031	7	0.038	0.004	0.000	0.041	7	0.011	0.011	0.000	0.021
	8	0.008	0.008	0.000	0.017	8	0.000	0.031	0.000	0.031	8	0.038	0.004	0.000	0.041	8	0.011	0.011	0.000	0.021
	9	0.008	0.008	0.000	0.017	9	0.000	0.031	0.000	0.031	9	0.038	0.004	0.000	0.041	9	0.011	0.011	0.000	0.021
	10	0.008	0.008	0.000	0.017	10	0.000	0.031	0.000	0.031	10	0.038	0.004	0.000	0.041	10	0.011	0.011	0.000	0.021
	tot	0.106	0.068	0.000	0.174	tot	0.000	0.308	0.000	0.308	tot	0.379	0.036	0.000	0.414	tot	0.107	0.107	0.000	0.214

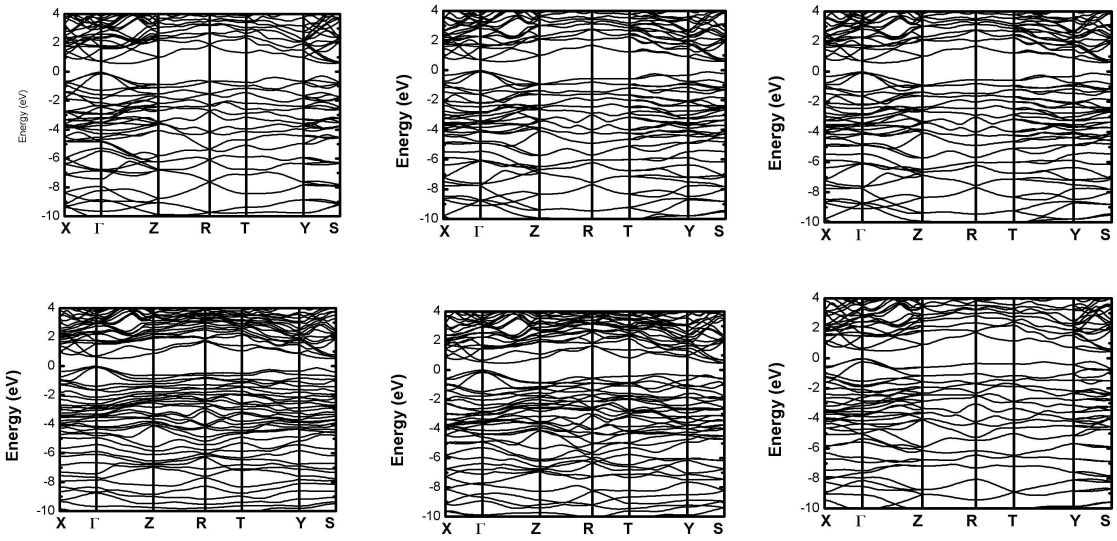
Special k-points	CBM					E					Line E-G					Line G-A				
VB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.000	0.043	0.000	0.043	1	0.000	0.057	0.000	0.057	1	0.002	0.041	0.000	0.044	1	0.000	0.044	0.000	0.044
	2	0.000	0.039	0.000	0.039	2	0.002	0.020	0.000	0.022	2	0.002	0.041	0.000	0.044	2	0.000	0.044	0.000	0.044
	3	0.000	0.059	0.000	0.060	3	0.001	0.029	0.000	0.030	3	0.002	0.041	0.000	0.044	3	0.000	0.044	0.000	0.044
	4	0.000	0.031	0.000	0.032	4	0.000	0.050	0.000	0.050	4	0.002	0.041	0.000	0.044	4	0.000	0.044	0.000	0.044
	5	0.000	0.030	0.000	0.030	5	0.001	0.039	0.000	0.040	5	0.002	0.041	0.000	0.044	5	0.000	0.044	0.000	0.044
	6	0.000	0.043	0.000	0.043	6	0.000	0.056	0.000	0.056	6	0.002	0.041	0.000	0.044	6	0.000	0.044	0.000	0.044
	7	0.000	0.040	0.000	0.040	7	0.002	0.023	0.000	0.025	7	0.002	0.041	0.000	0.044	7	0.000	0.044	0.000	0.044
	8	0.000	0.059	0.000	0.059	8	0.002	0.026	0.000	0.028	8	0.002	0.041	0.000	0.044	8	0.000	0.044	0.000	0.044
	9	0.000	0.031	0.000	0.031	9	0.000	0.049	0.000	0.049	9	0.002	0.041	0.000	0.044	9	0.000	0.044	0.000	0.044
	10	0.000	0.031	0.000	0.031	10	0.001	0.040	0.000	0.041	10	0.002	0.041	0.000	0.044	10	0.000	0.044	0.000	0.044
	tot	0.002	0.406	0.000	0.407	tot	0.010	0.389	0.000	0.399	tot	0.024	0.411	0.000	0.435	tot	0.003	0.441	0.000	0.444
CB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.011	0.008	0.000	0.019	1	0.010	0.007	0.000	0.017	1	0.010	0.013	0.000	0.023	1	0.010	0.008	0.000	0.019
	2	0.011	0.008	0.000	0.019	2	0.010	0.007	0.000	0.017	2	0.010	0.013	0.000	0.023	2	0.010	0.008	0.000	0.019
	3	0.011	0.008	0.000	0.019	3	0.010	0.007	0.000	0.017	3	0.010	0.013	0.000	0.023	3	0.010	0.008	0.000	0.019
	4	0.011	0.008	0.000	0.019	4	0.010	0.007	0.000	0.017	4	0.010	0.013	0.000	0.023	4	0.010	0.008	0.000	0.019
	5	0.011	0.008	0.000	0.019	5	0.010	0.007	0.000	0.017	5	0.010	0.013	0.000	0.023	5	0.010	0.008	0.000	0.019
	6	0.011	0.008	0.000	0.019	6	0.011	0.006	0.000	0.018	6	0.010	0.013	0.000	0.023	6	0.010	0.008	0.000	0.019
	7	0.011	0.008	0.000	0.019	7	0.011	0.006	0.000	0.018	7	0.010	0.013	0.000	0.023	7	0.010	0.008	0.000	0.019
	8	0.011	0.008	0.000	0.019	8	0.011	0.006	0.000	0.018	8	0.010	0.013	0.000	0.023	8	0.010	0.008	0.000	0.019
	9	0.011	0.008	0.000	0.019	9	0.011	0.006	0.000	0.018	9	0.010	0.013	0.000	0.023	9	0.010	0.008	0.000	0.019
	10	0.011	0.008	0.000	0.019	10	0.011	0.006	0.000	0.018	10	0.010	0.013	0.000	0.023	10	0.010	0.008	0.000	0.019
	tot	0.110	0.084	0.000	0.194	tot	0.106	0.068	0.000	0.174	tot	0.098	0.128	0.000	0.226	tot	0.104	0.085	0.000	0.189

Cc-Si_3AlP cell

Special k-points	Z					G					X					K				
VB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.001	0.056	0.000	0.057	1	0.000	0.043	0.000	0.043	1	0.009	0.035	0.000	0.044	1	0.004	0.037	0.000	0.041
	2	0.002	0.044	0.000	0.045	2	0.002	0.042	0.000	0.044	2	0.001	0.067	0.000	0.068	2	0.007	0.021	0.000	0.029
	3	0.000	0.005	0.000	0.006	3	0.001	0.042	0.000	0.042	3	0.001	0.034	0.000	0.035	3	0.002	0.070	0.000	0.072
	4	0.004	0.035	0.000	0.039	4	0.000	0.043	0.000	0.043	4	0.009	0.037	0.000	0.045	4	0.004	0.037	0.000	0.041
	5	0.005	0.013	0.000	0.018	5	0.002	0.042	0.000	0.044	5	0.003	0.015	0.000	0.018	5	0.007	0.021	0.000	0.029
	6	0.002	0.092	0.000	0.094	6	0.001	0.042	0.000	0.042	6	0.000	0.089	0.000	0.089	6	0.002	0.070	0.000	0.072
	7	0.008	0.025	0.000	0.033	7	0.000	0.028	0.000	0.028	7	0.000	0.033	0.000	0.033	7	0.000	0.039	0.000	0.039
	8	0.002	0.034	0.000	0.036	8	0.000	0.028	0.000	0.028	8	0.000	0.034	0.000	0.034	8	0.000	0.039	0.000	0.039
	9	0.002	0.011	0.000	0.013	9	0.000	0.048	0.000	0.048	9	0.000	0.009	0.000	0.009	9	0.002	0.004	0.000	0.006
	10	0.000	0.051	0.000	0.052	10	0.000	0.048	0.000	0.048	10	0.002	0.006	0.000	0.008	10	0.002	0.004	0.000	0.006
	tot	0.026	0.367	0.000	0.393	tot	0.006	0.406	0.000	0.412	tot	0.026	0.357	0.000	0.383	tot	0.030	0.345	0.000	0.375
CB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.002	0.015	0.000	0.017	1	0.019	0.028	0.000	0.047	1	0.021	0.005	0.000	0.026	1	0.010	0.016	0.000	0.026
	2	0.003	0.011	0.000	0.014	2	0.033	0.026	0.000	0.059	2	0.033	0.014	0.000	0.048	2	0.010	0.014	0.000	0.024
	3	0.006	0.013	0.000	0.019	3	0.003	0.009	0.000	0.012	3	0.031	0.007	0.000	0.038	3	0.009	0.017	0.000	0.025
	4	0.024	0.002	0.000	0.025	4	0.019	0.028	0.000	0.047	4	0.031	0.018	0.000	0.049	4	0.010	0.016	0.000	0.026
	5	0.016	0.004	0.000	0.020	5	0.033	0.026	0.000	0.059	5	0.015	0.007	0.000	0.021	5	0.010	0.014	0.000	0.024
	6	0.012	0.003	0.000	0.016	6	0.003	0.009	0.000	0.012	6	0.016	0.013	0.000	0.030	6	0.009	0.017	0.000	0.025
	7	0.013	0.003	0.000	0.016	7	0.002	0.005	0.000	0.006	7	0.028	0.005	0.000	0.033	7	0.003	0.011	0.000	0.014
	8	0.003	0.008	0.000	0.011	8	0.002	0.005	0.000	0.006	8	0.013	0.012	0.000	0.025	8	0.003	0.011	0.000	0.014
	9	0.004	0.017	0.000	0.021	9	0.029	0.046	0.000	0.075	9	0.045	0.004	0.000	0.048	9	0.012	0.008	0.000	0.020
	10	0.018	0.006	0.000	0.024	10	0.029	0.046	0.000	0.075	10	0.048	0.007	0.000	0.055	10	0.012	0.008	0.000	0.020
	tot	0.101	0.082	0.000	0.184	tot	0.172	0.226	0.000	0.398	tot	0.280	0.092	0.000	0.372	tot	0.088	0.131	0.000	0.220

Special k-points	CBM					E					Line E-G					Line G-A				
VB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.002	0.070	0.000	0.071	1	0.001	0.051	0.000	0.052	1	0.002	0.048	0.000	0.049	1	0.002	0.028	0.000	0.029
	2	0.004	0.020	0.000	0.024	2	0.006	0.011	0.000	0.017	2	0.006	0.024	0.000	0.030	2	0.003	0.058	0.000	0.061
	3	0.003	0.043	0.000	0.046	3	0.000	0.051	0.000	0.051	3	0.001	0.041	0.000	0.042	3	0.000	0.054	0.000	0.054
	4	0.002	0.070	0.000	0.071	4	0.001	0.051	0.000	0.052	4	0.002	0.048	0.000	0.049	4	0.000	0.057	0.000	0.057
	5	0.004	0.020	0.000	0.024	5	0.006	0.011	0.000	0.017	5	0.006	0.024	0.000	0.030	5	0.001	0.029	0.000	0.031
	6	0.003	0.043	0.000	0.046	6	0.000	0.051	0.000	0.051	6	0.001	0.041	0.000	0.042	6	0.002	0.030	0.000	0.032
	7	0.000	0.037	0.000	0.038	7	0.001	0.040	0.000	0.041	7	0.000	0.039	0.000	0.039	7	0.000	0.028	0.000	0.028
	8	0.000	0.037	0.000	0.038	8	0.001	0.040	0.000	0.041	8	0.000	0.039	0.000	0.039	8	0.002	0.021	0.000	0.023
	9	0.004	0.001	0.000	0.005	9	0.006	0.006	0.000	0.012	9	0.003	0.025	0.000	0.028	9	0.000	0.047	0.000	0.047
	10	0.004	0.001	0.000	0.005	10	0.006	0.006	0.000	0.012	10	0.003	0.025	0.000	0.028	10	0.002	0.047	0.000	0.048
	tot	0.025	0.342	0.000	0.367	tot	0.028	0.317	0.000	0.345	tot	0.023	0.353	0.000	0.376	tot	0.012	0.399	0.000	0.411
CB	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot	ion	s	p	d	tot
	1	0.010	0.014	0.000	0.023	1	0.009	0.013	0.000	0.022	1	0.010	0.015	0.000	0.025	1	0.011	0.016	0.000	0.027
	2	0.010	0.011	0.000	0.021	2	0.007	0.012	0.000	0.019	2	0.010	0.011	0.000	0.021	2	0.013	0.009	0.000	0.022
	3	0.009	0.015	0.000	0.024	3	0.010	0.006	0.000	0.016	3	0.009	0.016	0.000	0.026	3	0.005	0.007	0.000	0.012
	4	0.010	0.014	0.000	0.023	4	0.009	0.013	0.000	0.022	4	0.010	0.015	0.000	0.025	4	0.009	0.010	0.000	0.019
	5	0.010	0.011	0.000	0.021	5	0.007	0.012	0.000	0.019	5	0.010	0.011	0.000	0.021	5	0.011	0.011	0.000	0.021
	6	0.009	0.015	0.000	0.024	6	0.010	0.006	0.000	0.016	6	0.009	0.016	0.000	0.026	6	0.004	0.010	0.000	0.014
	7	0.004	0.012	0.000	0.016	7	0.012	0.009	0.000	0.020	7	0.013	0.015	0.000	0.028	7	0.007	0.008	0.000	0.016
	8	0.004	0.012	0.000	0.016	8	0.012	0.009	0.000	0.020	8	0.013	0.015	0.000	0.028	8	0.007	0.008	0.000	0.015
	9	0.012	0.006	0.000	0.018	9	0.010	0.003	0.000	0.013	9	0.005	0.010	0.000	0.015	9	0.018	0.013	0.000	0.031
	10	0.012	0.006	0.000	0.018	10	0.010	0.003	0.000	0.013	10	0.005	0.010	0.000	0.015	10	0.015	0.015	0.000	0.031
	tot	0.088	0.117	0.000	0.204	tot	0.094	0.086	0.000	0.180	tot	0.094	0.134	0.000	0.228	tot	0.101	0.109	0.000	0.209

XI. Band structures of the six 20-atoms structures (same order as in Figure 2)



As we can see, the band structures of the structures with different arrangements of the basic unit [Si_3AlP] are almost the same, indicating that as long as the basic motif is the same, the band gaps are not sensitive to the atomic arrangements, which offers convenience for the experiment. This can be easily understood since the band folding relationships and the local chemical environment are the same.

XII. Structural and energy information of relaxed Cc, superlattice, and $P1_1$ to $P1_5$ structures

1. Cc primitive cell and superlattice structure

	Cc (primitive)	superlattice
Relaxed energy (Hartree/atom)	-0.2085146	-0.2139194
Relaxed atomic positions	Si Al P 5.40257000000000 1.0066964650592214 -0.5056785178695579 0.5010704755550753 1.0066964650592214 0.5056785178695579 0.5010704755550753 -1.5083734565946452 0.0000000000000000 0.4977307071733382 6 2 2 Direct 0.4010825316708377 0.4135639303793042 0.1981428140487651 0.7802397504655261 0.8463083241881790 0.4113648059737045 0.0228493080534307 0.9959696302532564 0.0097126586674179 0.1435639303793081 0.6710825316708338 0.6981428140487651 0.5763083241881830 0.0502397504655221 0.9113648059737045 0.7259696302532532 0.2928493080534338 0.5097126586674179 0.9359647647685421 0.4757842370491900 0.1019143128771276 0.2057842370491869 0.2059647647685452 0.6019143128771276 0.5770849615558973 0.6311525616158420 0.7988654084329738 0.3611525616158389 0.8470849615559004 0.2988654084329738	Si Al P 1.00000000000000 -2.7071592416448516 2.7071592416448516 0.0000000000000000 -2.7071592416448516 0.0000000000000000 -2.7071592416448516 -10.8673537493067336 -8.1601945076618829 8.1601945076618829 6 2 2 Direct 0.9998218661326490 0.9998218661326490 0.0005344016020530 0.3495632199660363 0.3495632199640326 0.9513103401049108 0.3992785070982379 0.3992785070982379 0.8021644787052793 0.7490693728910145 0.7490693728890108 0.7527918813299621 0.7987655530861133 0.7987655530861133 0.6037033407416459 0.1486292090544339 0.1486292090524302 0.5541123728396968 0.2005487832709392 0.2005487832709392 0.3983536501871754 0.6009087854322814 0.6009087854322814 0.1972736437031770 0.5516465447254433 0.5516465447234467 0.3450603658266616 0.9517681583478534 0.9517681583458568 0.1446955249594311

2. Cc conventional cell and $P1_1$ structures

	Cc	$P1_1$
Relaxed energy (Hartree/atom)	-0.2085146	-0.2079947
Relaxed atomic positions	Si Al P 1.00000000000000 8.5807165173050759 0.0255343741861376 0.0000009634865445 0.0254911639914040 8.5500079180329731 0.0000008188459229 0.0000000555325108 -0.0000007246842219 5.4643111510166333 12 4 4 Direct 0.5005707868013829 0.0078693727597141 0.2270022389641397 0.8077937760848073 0.1019205515663870 0.7537697665498655 0.0005536077957302 0.0078759368342105 0.0229910734994192 0.3078080044008544 0.1019206393888084 0.4962155109438271 0.0983222126781413 0.2040669955841423 0.2734642069327151 0.0005666669960434 0.5078896037063458 0.7270251760437532 0.3078027606397029 0.6019100787883858 0.2537831286416363 0.5983116537676523 0.2040710992120438 0.9765224244727335 0.5005838873675330 0.5078832070198587 0.5229814931475119 0.8077883067030456 0.6019101530047735 0.9962315994759692 0.5983189166308165 0.7040832980382987 0.7734715939588597 0.0983293707316122 0.7040790935745704 0.4765416752528751 0.2025398505936806 0.4004781825816082 0.9901077443191824 0.7025524710485200 0.4004593484696670 0.2598994544337430 0.2025383393917650 0.9004973499157174 0.7598962481135985 0.7025509021885341 0.9004787543251496 0.4900965092676515 0.4038588213389573 0.2987555744222945 0.7330087814397643 0.9038750920812575 0.2987472121887222 0.5169928413426845 0.9038654291742603 0.7987325896439472 0.2330212475383888 0.4038491435857026 0.7987409589753369 0.0169772856616817	Si Al P 1.00000000000000 8.5705502882058404 0.0000000000000000 0.0000000000000000 0.0000000000000000 8.5705137887544875 0.0000000000000000 0.0000000000000000 0.0000000000000000 5.4524291404590155 12 4 4 Direct 0.5047003208886025 0.0043061022448683 0.2177494791508678 0.8005387323545818 0.1009289995811002 0.7177470564310866 0.1008556511421688 0.2102058419777606 0.2643314439997653 0.0042106356703684 0.5028066886749301 0.7521228082050300 0.3010288551244500 0.6024318867731751 0.2521238090060436 0.6043069297741823 0.2005342137422730 0.9677450683612250 0.4950319397189418 0.5008590326903715 0.5143322235458427 0.8102095010710713 0.6043779239604987 0.0143326605814025 0.1028065367826869 0.7010295861397893 0.5021221894872738 0.2024303788680299 0.4042082416552262 0.0021257314974790 0.2043785326207299 0.8950317824505802 0.7643307459631430 0.7009319858394178 0.9046996264860283 0.4677462101334129 0.3096184524512111 0.1006953845337435 0.5070067186998344 0.7006954917202890 0.3956153007837528 0.2570072494776525 0.9956172556926575 0.0045412963224436 0.0070078559798503 0.6045447240494610 0.7096142138036200 0.7570115368448924 0.3983483647658161 0.3071430161734341 0.7587898441741459 0.9071428993493242 0.3068885180730234 0.5087907684318722 0.9068888147074787 0.7980951475436768 0.2587887932694741 0.3980939974085160 0.7983499888129444 0.0087878067597202

3. $P1_2$ and $P1_3$ structures

	$P1_2$	$P1_3$
Relaxed energy (Hartree/atom)	-0.2079946	-0.2079178
Relaxed atomic positions	Si Al P 1.00000000000000 8.5699235688503812 -0.0000027129412904 -0.0000218882567377 -0.0000004264601075 8.5698993942449473 0.0000101643987910 -0.0000141340954601 0.0000065143236870 5.4518813519390648 12 4 4 Direct 0.4949617731733227 0.0008366213903486 0.2357215428743515 0.8102647673086594 0.1044123653550955 0.7357315681288625 0.0042090345714598 0.0027932519888481 0.9979057167772822 0.3010371628031905 0.1024549368669625 0.4979156839639742 0.1027974916430949 0.2010351948232909 0.2479108391709062 0.5047089442869463 0.5042834867436241 0.5321595988242862 0.8005183994591505 0.6009403387710961 0.0321571473419340 0.6042814438072455 0.7005195189172966 0.7821554805188455 0.1008504522534324 0.7102670401476630 0.4857272511733939 0.2044039863825446 0.3949682287784952 0.9857253832806663 0.7009427140934363 0.4047062444283966 0.2821607783291711 0.2024568800302404 0.9042074765642454 0.7479064675606111 0.6045190665743334 0.2095590230949043 0.9930281678303885 0.9956869509344060 0.5045342668210679 0.7430279461723472 0.7007014850024831 0.8956842488188101 0.4930281369177223 0.3095645909727054 0.6006936711274449 0.2430221056011916 0.3980908879971850 0.2983557411457980 0.7411778711768306 0.9068869794770720 0.2980973906915025 0.4911729384933139 0.9071506906238298 0.8068818476439859 0.2411784232694885 0.3983462986052757 0.8071391058811486 0.9911869525944326	Si Al P 1.00000000000000 8.5521075435636202 -0.0073050614262203 0.0013765880652257 -0.0073200796149963 8.5809881294659061 -0.0077117961866391 0.0008783877560087 -0.0049045290241338 5.4622336213478873 12 4 4 Direct 0.5041929951383537 0.0038296632150931 0.2240012079435232 0.8008307457738226 0.1045694927408789 0.7159187696111218 0.1013118962615422 0.2081531151691962 0.2593730929456655 0.3037637058849469 0.6023884118229716 0.2486361075621986 0.6083347822849845 0.2036928012311279 0.9759301303677717 0.5006952299783478 0.4990054836915334 0.5122202903240307 0.8045800987106588 0.6034298933126578 0.0329854664672524 0.1044928557993714 0.7038916972297571 0.4958878305034489 0.2058233094203175 0.4030627265479296 0.9993522146345768 0.6974599180576249 0.3970099323428187 0.2560379093200638 0.2059047858808754 0.8943558703213910 0.7613064927792337 0.6996552567805239 0.9037394206479803 0.4783316312186017 0.3075394304682959 0.1023551316452327 0.5133162187245546 0.9978698497997911 0.5014720429048793 0.7477443312570742 0.9973974651616686 0.0034227171439198 0.9991888214464879 0.6071368303873470 0.7062335433941129 0.7634350227208486 0.4048253471540377 0.3065155588727535 0.7631990442906087 0.8969368610570640 0.3034878208963221 0.4878913880136508 0.9041900453347935 0.8024495156508635 0.2611960287064790 0.3994385906656390 0.7993051612185980 0.0040480011628290

4. $P1_4$ and $P1_5$ structures

	$P1_4$	$P1_5$
Relaxed energy (Hartree/atom)	-0.2078771	-0.2078117
Relaxed atomic positions	Si Al P 1.00000000000000 8.5649365675647875 -0.0183073675755205 -0.0000070668810263 -0.0182769354634959 8.5554979382128984 0.0000019485983528 -0.0000044681883739 0.0000019284959099 5.4723752122369405 12 4 4 Direct 0.5001277870641161 0.0033944185607240 0.2351998884610822 0.0001239116733842 0.0033966334530930 0.0147983902490409 0.1031829674758242 0.2053420196352675 0.2616033572177869 0.9997908456264923 0.4993382474924033 0.7446355133858162 0.3037282268219386 0.5988149609823950 0.2433500659638881 0.6031793191489285 0.2053431184435368 0.9883963662573478 0.4997940644124341 0.4993377542970308 0.5053666740501157 0.8037242749227431 0.5988143907167469 0.0066500812828778 0.2012636727514661 0.4003180088553506 0.9895928752666521 0.7012654993646379 0.4003156031670017 0.2604094698930268 0.2028236350119954 0.9012316158001070 0.7887746375350346 0.7028258870244954 0.9012258441186773 0.4612226319358328 0.3057440261407081 0.0995044657458806 0.5238522905357144 0.8057371154968180 0.0995047815251056 0.7261439950596298 0.1028542644153987 0.7092544367359324 0.5031792212466897 0.6028491308171411 0.7092566527061592 0.7468247492900133 0.4044474838318806 0.3081528833221370 0.7586772110766589 0.9044512533457763 0.3081507592978738 0.4913232528457030 0.9022354038738101 0.8008350413296910 0.2419400356185548 0.4022312307799893 0.8008383638148970 0.0080592928285128	Si Al P 1.00000000000000 8.5620383559265107 -0.0287155117232978 -0.0000061640142410 -0.0287703419188870 8.5927309108795100 -0.0000063899577137 -0.0000043780965054 -0.0000037946536270 5.4494432379146547 12 4 4 Direct 0.5037067764947878 0.9997848273045591 0.2229900426230955 0.8015302702918419 0.1054557876868003 0.7229939740970579 0.0993405316449198 0.2081035030567833 0.2576978776029151 0.6091797192601049 0.2044251065431339 0.9868065916014217 0.5037143422193964 0.4998053298993810 0.5269862313711045 0.8015227005263696 0.6054300518014557 0.0269937574179551 0.6091844013914738 0.7044383253644781 0.7631856573107285 0.0993691022917886 0.7081478135426593 0.4923182742391958 0.2058804389212767 0.3970883762698705 0.9923012333152883 0.6960480674448277 0.4007941867629654 0.2631796652523448 0.2059028004128649 0.8971412984452911 0.7577091502149855 0.6960504648109094 0.9008134870727176 0.4868184279947485 0.3056317569934563 0.1033106929514318 0.5053504360203718 0.9996374740770051 0.5019627911832956 0.7446455444553948 0.9996032981857255 0.0019241532705436 0.0053627463591610 0.3056026996279329 0.6032713133065215 0.2446401268979912 0.4083217687729359 0.3017783559801615 0.7645762645020042 0.8969302782701902 0.3034925768011902 0.4854175810493189 0.8969158563820159 0.8034560314117627 0.2645998520326529 0.4083072519801547 0.8017459913449869 0.9854265656422427