Electronic Supplementary Material (ESI) for RSC Advances.

Atom	WIEN2k			VASP		
1	0.005925	-0.001520	0.000151	0.008027	0.001037	-0.002668
2	-0.005956	0.001495	-0.000180	-0.008027	-0.001037	0.002668
3	0.005896	-0.001383	0.000385	0.008027	0.001037	0.002668
4	-0.005912	0.001457	-0.000380	-0.008027	-0.001037	-0.002668
5	-0.005896	-0.001383	0.000386	-0.008027	0.001037	0.002668
6	0.005909	0.001457	-0.000380	0.008027	-0.001037	-0.002668
7	-0.005926	-0.001520	0.000149	-0.008027	0.001037	-0.002668
8	0.005955	0.001494	-0.000180	0.008027	-0.001037	0.002668
9	0.000743	-0.004953	-0.000924	0.000267	0.006880	0.013629
10	-0.000763	0.005019	0.001157	-0.000267	-0.006880	-0.013629
11	-0.000835	0.005160	-0.001500	-0.000267	-0.006880	0.013629
12	0.000820	-0.005147	0.001276	0.000267	0.006880	-0.013629
13	0.000836	0.005160	-0.001500	0.000267	-0.006880	0.013629
14	-0.000819	-0.005147	0.001277	-0.000267	0.006880	-0.013629
15	-0.000744	-0.004954	-0.000923	-0.000267	0.006880	0.013629
16	0.000763	0.005018	0.001157	0.000267	-0.006880	-0.013629
17	0.000003	0.014742	-0.008537	0.000000	0.010455	-0.013294
18	-0.000002	-0.014785	0.008705	0.000000	-0.010455	0.013294
19	-0.000003	-0.014726	-0.008002	0.000000	-0.010455	-0.013294
20	0.000003	0.014748	0.007848	0.000000	0.010455	0.013294
21	0.007840	-0.000105	0.002707	0.008298	-0.003831	-0.002533
22	-0.007870	0.000185	-0.002486	-0.008298	0.003831	0.002533
23	0.007764	-0.000349	-0.001321	0.008298	-0.003831	0.002533
24	-0.007812	0.000249	0.001123	-0.008298	0.003831	-0.002533
25	-0.007762	-0.000351	-0.001322	-0.008298	-0.003831	0.002533
26	0.007809	0.000249	0.001122	0.008298	0.003831	-0.002533
27	-0.007836	-0.000107	0.002706	-0.008298	-0.003831	-0.002533
28	0.007866	0.000185	-0.002487	0.008298	0.003831	0.002533
29	0.000003	-0.002381	0.003017	0.000000	-0.010734	0.008233
30	-0.000004	0.002295	-0.002543	0.000000	0.010734	-0.008233
31	0.000004	-0.002089	-0.001789	0.000000	-0.010734	-0.008233
32	-0.000004	0.002246	0.001315	0.000000	0.010734	0.008233
33	0.000003	0.005342	0.000694	0.000000	-0.003883	-0.001434
34	-0.000003	-0.005593	-0.001325	0.000000	0.003883	0.001434
35	0.000003	0.005212	-0.000098	0.000000	-0.003883	0.001434
36	-0.000003	-0.005309	0.000681	0.000000	0.003883	-0.001434
37	0.000004	-0.001531	0.005020	0.000000	0.005800	0.002359
38	-0.000003	0.001580	-0.004740	0.000000	-0.005800	-0.002359
39	-0.000004	0.001858	0.006515	0.000000	-0.005800	0.002359
40	0.000003	-0.001955	-0.006825	0.000000	0.005800	-0.002359
41	-0.000004	0.011224	0.014197	0.000000	0.010617	0.001421
42	0.000003	-0.011012	-0.014007	0.000000	-0.010617	-0.001421
43	-0.000003	0.011057	-0.012885	0.000000	0.010617	-0.001421
44	0.000003	-0.011029	0.012691	0.000000	-0.010617	0.001421
45	0.000000	0.006996	0.005341	0.000000	0.004640	0.009054
46	0.000000	-0.007004	-0.005150	0.000000	-0.004640	-0.009054

47	0.000000	0.007068	-0.005513	0.000000	0.004640	-0.009054
48	0.000000	-0.007075	0.005368	0.000000	-0.004640	0.009054
49	-0.000001	-0.009036	0.008030	0.000000	-0.000079	0.005393
50	0.000000	0.008961	-0.008441	0.000000	0.000079	-0.005393
51	-0.000001	-0.008633	-0.007628	0.000000	-0.000079	-0.005393
52	0.000001	0.008570	0.008038	0.000000	0.000079	0.005393

Table S1 The calculated forces on each atom of the optimized structure Sr5Al2Sb6 by WIEN2k and VASP