Supplementary Information:

Mg_9Si_5 crystallizes in the hexagonal structure with space group symmetry $P6_3$ (space group No. 173). The lattice parameters a= 12.411Åand c= 12.345Å are taken from the experiments. The GGA optimized coordinates of Mg_9Si_5 are given below, which is compared with experimental data of Ref. 38 of the revised manuscript.

		Expterimental			Optimized structure		
	Site	x	y	z	x	y	z
Mg	6c	0.2433	0.1698	0.2526	0.2430	0.1701	0.2884
Mg	6c	0.5335	0.4047	0.2541	0.5327	0.4041	0.7875
Mg	6c	0.0773	0.2331	0.0939	0.0701	0.2129	0.6264
Mg	6c	0.8270	0.2528	0.0793	0.8276	0.2534	0.1145
Mg	6c	0.4982	0.5894	0.0901	0.5007	0.5910	0.1228
Mg	6c	0.2656	0.4566	0.2558	0.2659	0.4570	0.2864
Mg	6c	0.2539	0.4259	-0.0730	0.2523	0.4243	0.9611
Mg	6c	0.4995	0.4089	-0.0811	0.5008	0.4108	0.9513
Mg	6c	0.0721	0.2132	0.4141	0.0774	0.2352	0.4474
Si	2a	0.000	0.000	0.0436	0.000	0.000	0.00258
Si	2a	0.000	0.000	-0.0338	—	—	—
Si	2a	0.000	0.000	0.2492	0.000	0.000	0.29935
Si	6c	0.3310	0.0037	0.2556	0.3315	0.0040	0.2858
Si	2b	0.3333	0.6667	-0.0951	0.3333	0.6667	0.9381
Si	6c	0.3363	0.3353	0.4195	0.3359	0.3362	0.4519
Si	6c	0.3358	0.3358	0.0896	0.3359	0.3356	0.1224
Si	2b	0.3333	0.6667	0.1080	0.3333	0.6667	0.1404
Si	2b	0.6667	0.3333	-0.0970	0.6667	0.3333	0.9363
Si	2b	0.6667	0.3333	0.1057	0.6667	0.3333	0.6386