Electronic Supplementary Information

Effects of doping atoms (Sb, Te, Sn, P and Bi) on the equilibrium shape of Mg_2Si from first-principles calculations

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Table S1 The percentage of the change of the interlayer spacing for the relaxed Mg_2Si (100) slabs relative to the bulk spacing.

Termination	**Change in interlayer**	**Slab thickness (*N*)**		
		5(%)	9(%)	13(%)
Si	$\Delta d1-2$	-10.10	-10.79	-7.78
	$\Delta d2-3$	4.96	5.90	5.08
	$\Delta d3-4$		0.69	-1.07
	$\Delta d4-5$		0.56	2.45
	$\Delta d5-6$			-1.76
	$\Delta d6-7$			-0.69
		7(%)	11(%)	15(%)
Mg	$\Delta d1-2$	-0.63	-0.94	-1.51
	$\Delta d2-3$	1.76	1.82	2.01
	$\Delta d3-4$	-0.13	-0.56	-0.56
	$\Delta d4-5$		0.56	1.32
	$\Delta d5-6$		0.38	-0.19
	$\Delta d6-7$			0.13
	$\Delta d7-8$			0.63

Table S2 The percentage of the change of the interlayer spacing for the relaxed Mg_2Si (111) slabs relative to the bulk interlayer spacing.

Termination	Change in interlayer	Slab thickness (*N*)		
		6(%)	9(%)	12(%)
Mg-I	$\Delta d1-2$	-31.85	-24.46	-31.09
	$\Delta d2-3$	15.22	8.37	12.07
	$\Delta d3-4$	-5.98	-2.28	-2.55
	$\Delta d4-5$		0.00	4.57
	$\Delta d5-6$			-1.85
	$\Delta d6-7$			2.34
		8(%)	11(%)	14(%)
Mg-II	$\Delta d1-2$	-1.85	-0.76	-3.42
	$\Delta d2-3$	3.70	2.39	4.02
	$\Delta d3-4$	1.74	4.89	0.43
	$\Delta d4-5$	0.00	1.20	0.43
	$\Delta d5-6$		2.39	0.00
	$\Delta d6-7$			0.76
	$\Delta d7-8$			0.60
		7(%)	10(%)	13(%)
Si	$\Delta d1-2$	-34.24	-35.98	-18.48
	$\Delta d2-3$	12.93	14.62	6.47
	$\Delta d3-4$	1.96	0.11	4.57
	$\Delta d4-5$		4.46	-2.83
	$\Delta d5-6$		0.76	1.25
	$\Delta d6-7$			2.28

Fabrication procedure of Al-20 wt.% Mg_2Si alloy

The Al-12.6 wt.% Si alloy was prepared at 750 ^{o}C in a graphite crucible. Pure Mg preheated at 200 ^{o}C in a resistance furnace was then added to the molten alloys. The melts were manually stirred for about 2 min, held at 750 ^{o}C for 20 min. Then the molten alloys was poured to a metal mold preheated at 150 ^{o}C to produce ingots Al-20 wt.% Mg_2Si alloys. The Al-20 wt.% Mg_2Si alloys were remelted at 800 ^{o}C, and then designed contents of the modifiers (pure Sn (99.90 wt.%, purity), pure Te (99.00 wt.%, purity) and Al-3P master alloy) were added to the melts to get experimental alloys. The detailed fabrication procedure was reported elsewhere.[8]