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Supplementary information

In the following we list the structural data and formation energies for binary Mo-Si alloys (Tab. 1) and Ru-Si alloys (Tab. 2) which are stable with respect to decomposition into the elements ($E_f < 0$) according to our final PAW calculations.

Si content	composition	structure type	a[Å]	b[Å]	c[Å]	E_f [eV/atom]
0.250	Mo12Si4	Fe3C,oP16,62	6.11	7.89	5.03	-0.086
0.250	Mo12Si4	Ni3P,tI32,82	7.42	7.42	7.42	-0.233
0.250	Mo24Si8	Ti3P,tP32,86	9.84	9.84	4.94	-0.220
0.250	Mo3Si1	BiF3,cF16,225	4.37	4.37	4.37	-0.066
0.250	Mo6Si2	Cr3Si,cP8,223	4.89	4.89	4.89	-0.345
0.250	Mo6Si2	Mg3Cd,hP8,194	5.40	5.40	4.71	-0.085
0.250	Mo6Si2	Pt3Ge,mS16,12	5.36	5.36	6.04	-0.039
0.265	Mo25Si9	Pd25Ge9,hP34,147	7.17	7.17	11.43	-0.111
0.279	Mo31Si12	Ni31Si12,hP43,150	7.21	7.21	14.27	-0.096
0.294	Mo12Si5	Ni12P5,tI34,87	7.55	7.55	7.55	-0.117
0.294	Mo48Si20	Pt12Si5,tP68,85	14.21	14.21	5.10	-0.119
0.333	Mo16Si8	Re2Si,mP24,14	6.45	10.14	5.46	-0.109
0.333	Mo4Si2	Co1.75Ge,hP6,194	4.46	4.46	5.09	-0.070
0.333	Mo4Si2	CuAl2,tI12,140	4.87	4.87	4.87	-0.314
0.333	Mo4Si2	Ni2Al,hP6,164	4.40	4.40	5.20	-0.108
0.333	Mo6Si3	Fe2P,hP9,189	6.92	6.92	3.18	-0.264
0.333	Mo8Si4	Co2Si-b,oP12,62	5.30	4.18	7.97	-0.127
0.375	Mo10Si6	Cr5B3,tI32,140	7.28	7.28	7.28	-0.263
0.375	Mo10Si6	Mn5Si3,hP16,193	7.30	7.30	5.04	-0.311
0.375	Mo10Si6	Rh5Ge3,oP16,55	5.79	9.64	4.24	-0.151
0.375	Mo10Si6	W5Si3,tI32,140	7.27	7.27	7.27	-0.407
0.400	Mo24Si16	Ni3Si2,oS80,36	8.97	8.97	7.56	-0.120
0.400	Mo6Si4	U3Si2,tP10,127	6.62	6.62	3.28	-0.263
0.429	Mo16Si12	Ru4Si3,oP28,62	5.32	4.27	17.72	-0.118
0.444	Mo20Si16	Gd5(Ge0.5Si0.5)4,mP36,14	12.43	6.83	6.16	-0.281
0.444	Mo20Si16	Gd5Si4,oP36,62	6.16	12.43	6.83	-0.281
0.444	Mo20Si16	Sm5Ge4,oP36,62	6.16	12.43	6.83	-0.280
0.455	Mo12Si10	Pt6Si5,mP22,11	6.59	3.11	16.55	-0.148
0.455	Mo12Si10	V6Si5,oI44,72	9.32	9.32	9.32	-0.332
0.500	Mo1Si1	CsCl,cP2,221	3.04	3.04	3.04	-0.109
0.500	Mo2Si2	TlI,oS8,63	4.72	4.72	4.14	-0.345
0.500	Mo4Si4	FeAs,oP8,62	5.83	3.14	6.58	-0.258
0.500	Mo4Si4	FeB-b,oP8,62	5.75	4.16	4.74	-0.356
0.500	Mo4Si4	FeSi,cP8,198	4.87	4.87	4.87	-0.358
0.500	Mo4Si4	RhSi,mP8,14	4.75	4.78	5.67	-0.340
0.500	Mo4Si4	TiSi,oP8,25	4.28	6.12	4.30	-0.109
0.571	Mo12Si16	Rh3Si4,oP28,62	20.50	3.24	6.38	-0.253
0.600	Mo16Si24	Ru2Ge3,oP40,60	11.87	8.47	5.88	-0.172
0.600	Mo8Si12	Ru2Sn3,tP20,116	5.77	5.77	9.31	-0.121
0.625	Mo24Si40	Ir3Si5,mP64,14	6.90	13.66	12.55	-0.144
0.636	Mo16Si28	Mn4Si7,tP44,116	5.84	5.84	18.78	-0.354
0.667	Mo1Si2	Fe0.92Si2,tP3,123	3.02	3.02	5.25	-0.089
0.667	Mo1Si2	MoSi2,tI6,139	4.54	4.54	4.54	-0.506
0.667	Mo1Si2	ReSi2,oI6,71	4.54	4.54	4.54	-0.506
0.667	Mo2Si4	OsGe2,mS12,12	4.70	4.70	7.79	-0.111
0.667	Mo2Si4	TiSi2,oF24,70	4.95	5.95	4.64	-0.427
0.667	Mo2Si4	ZrSi2,oS12,63	7.18	7.18	3.42	-0.121
0.667	Mo3Si6	CrSi2,hP9,180	4.61	4.61	6.60	-0.478
0.667	Mo8Si16	FeSi2,oS48,64	6.75	6.75	8.14	-0.158

Table 1: Structural data and formation energy for binary Mo-Si alloys.
The assignment of the structure type refers to the initial trial structure

Si content	composition	structure type	a[Å]	b[Å]	c[Å]	E_f [eV/atom]
0.182	Ru36Si8	Pd9Si2,oP44,62	9.01	7.27	9.26	-0.086
0.250	Ru12Si4	Fe3C,oP16,62	5.33	7.58	5.44	-0.160
0.250	Ru12Si4	Ni3P,tI32,82	7.16	7.16	7.16	-0.229
0.250	Ru24Si8	Ti3P,tP32,86	9.57	9.57	4.78	-0.209
0.250	Ru6Si2	Ir3Si,tI16,140	5.41	5.41	5.41	-0.174
0.250	Ru6Si2	Mg3Cd,hP8,194	5.44	5.44	4.23	-0.071
0.250	Ru6Si2	Pt3Ge,mS16,12	5.28	5.28	5.41	-0.174
0.265	Ru25Si9	Pd25Ge9,hP34,147	7.19	7.19	10.30	-0.223
0.279	Ru31Si12	Ni31Si12,hP43,150	7.17	7.17	13.09	-0.245
0.294	Ru12Si5	Ni12P5,tI34,87	7.11	7.11	7.11	-0.231
0.333	Ru16Si8	Re2Si,mP24,14	6.32	9.56	5.32	-0.369
0.333	Ru2Si1	ThH2,tI6,139	3.99	3.99	3.99	-0.127
0.333	Ru4Si2	Co1.75Ge,hP6,194	4.18	4.18	5.35	-0.164
0.333	Ru4Si2	CuAl2,tI12,140	4.73	4.73	4.73	-0.279
0.333	Ru4Si2	Ni2Al,hP6,164	4.19	4.19	5.26	-0.199
0.333	Ru6Si3	Fe2P,hP9,189	6.10	6.10	3.83	-0.317
0.333	Ru8Si4	Co2Si-b,oP12,62	5.33	4.03	7.45	-0.398
0.375	Ru10Si6	Cr5B3,tI32,140	7.17	7.17	7.17	-0.352
0.375	Ru10Si6	Mn5Si3,hP16,193	6.89	6.89	5.26	-0.415
0.375	Ru10Si6	Rh5Ge3,oP16,55	5.30	9.89	4.04	-0.448
0.375	Ru10Si6	W5Si3,tI32,140	6.98	6.98	6.98	-0.386
0.400	Ru24Si16	Ni3Si2,oS80,36	8.78	8.78	7.29	-0.298
0.400	Ru3Si2	Ni2Al3,hP5,164	4.01	4.01	5.10	-0.335
0.400	Ru6Si4	U3Si2,tP10,127	6.05	6.05	3.71	-0.263
0.429	Ru16Si12	Ru4Si3,oP28,62	5.24	4.03	17.36	-0.541
0.444	Ru20Si16	Gd5(Ge0.5Si0.5)4,mP36,14	11.96	6.47	6.34	-0.467
0.444	Ru20Si16	Gd5Si4,oP36,62	6.35	11.97	6.46	-0.467
0.444	Ru20Si16	Sm5Ge4,oP36,62	6.35	11.98	6.44	-0.467
0.455	Ru12Si10	Pt6Si5,mP22,11	6.46	2.92	16.22	-0.423
0.455	Ru12Si10	V6Si5,oI44,72	8.76	8.76	8.76	-0.412
0.500	Ru1Si1	CsCl,cP2,221	2.94	2.94	2.94	-0.636
0.500	Ru2Si2	TlI,oS8,63	4.59	4.59	4.03	-0.492
0.500	Ru4Si4	FeAs,oP8,62	5.78	2.98	6.37	-0.563
0.500	Ru4Si4	FeB-b,oP8,62	5.88	4.16	4.16	-0.637
0.500	Ru4Si4	FeSi,cP8,198	4.74	4.74	4.74	-0.639
0.500	Ru4Si4	RhSi,mP8,14	4.62	4.67	5.46	-0.577
0.500	Ru4Si4	TiSi,oP8,25	4.15	5.89	4.17	-0.637
0.571	Ru12Si16	Rh3Si4,oP28,62	19.97	3.12	6.30	-0.543
0.600	Ru16Si24	Ru2Ge3,oP40,60	11.16	9.00	5.57	-0.625
0.600	Ru4Si6	Pt2Sn3,hP10,194	3.68	3.68	12.84	-0.310
0.600	Ru8Si12	Ru2Sn3,tP20,116	5.60	5.60	8.95	-0.603
0.625	Ru24Si40	Ir3Si5,mP64,14	6.39	13.96	11.91	-0.377
0.636	Ru16Si28	Mn4Si7,tP44,116	5.77	5.77	18.33	-0.354
0.667	Ru1Si2	CaF2,cF12,225	4.02	4.02	4.02	-0.241
0.667	Ru1Si2	Fe0.92Si2,tP3,123	2.88	2.88	5.27	-0.412
0.667	Ru1Si2	MoSi2,tI6,139	4.43	4.43	4.43	-0.236
0.667	Ru1Si2	ReSi2,oI6,71	4.43	4.43	4.43	-0.236
0.667	Ru2Si4	OsGe2,mS12,12	4.60	4.60	7.47	-0.508
0.667	Ru2Si4	TiSi2,oF24,70	5.18	6.08	4.45	-0.202
0.667	Ru2Si4	ZrSi2,oS12,63	6.18	6.18	3.75	-0.160
0.667	Ru3Si6	CrSi2,hP9,180	4.47	4.47	6.91	-0.194
0.667	Ru8Si16	FeSi2,oS48,64	6.52	6.52	8.23	-0.535

Table 2: Same as Tab. 1 for Ru-Si.

Mg content	composition	structure type	a[Å]	b[Å]	c[Å]	E_f [eV/atom]
0.500	Mg2Si2	TlI,oS8,63	5.42	5.42	3.65	-0.022
0.538	Mg28Si24	Ca7Sn6,oP52,62	6.53	20.62	7.30	-0.023
0.556	Mg20Si16	Sm5Ge4,oP36,62	6.60	14.45	7.21	-0.010
0.608	Mg62Si40	Pu31Pt20,tI204,140	18.72	18.72	18.72	-0.044
0.610	Mg72Si46	Yb36Sn23,tP118,127	10.56	10.56	20.02	-0.050
0.625	Mg10Si6	Cr5B3,tI32,140	8.35	8.35	8.35	-0.059
0.625	Mg10Si6	Sr5Si3,tI32,108	8.34	8.34	8.34	-0.059
0.625	Mg20Si12	Ba5Si3,tP32,130	6.75	6.75	13.71	-0.062
0.625	Mg30Si18	Ca5Pb3,hP48,186	13.61	13.61	5.82	-0.046
0.643	Mg18Si10	Mg9Si5,hP28,176	7.17	7.17	12.30	-0.120
0.667	Mg2Si1	CaF2,cF12,225	4.49	4.49	4.49	-0.162
0.667	Mg8Si4	Co2Si-b,oP12,62	7.05	4.18	8.03	-0.105
0.750	Mg3Si1	Cu3Au,cP4,221	4.25	4.25	4.25	-0.007

Table 3: Same as Tab. 1 for Mg-Si.

Mg content	composition	structure type	a[Å]	b[Å]	c[Å]	E_f [eV/atom]
0.333	Ge4Mg2	(Li0.1Ca0.9)(Li0.03Ge0.97)2,hP6,186	3.93	3.93	9.55	-0.019
0.400	Ge6Mg4	Sr2Pb3,tP10,127	7.08	7.08	4.04	-0.014
0.429	Ge24Mg18	Ca3Si4,hP42,176	8.05	8.05	15.69	-0.038
0.455	Ge6Mg5	Mg5Si6,mS22,12	8.34	8.34	7.03	-0.041
0.455	Ge6Mg5	Mg5Si6,mS22,8	8.37	8.37	7.05	-0.041
0.500	Ge10Mg10	SrSi,oI40,71	10.52	10.52	10.52	-0.052
0.500	Ge1Mg1	CuAu,tP2,123	3.12	3.12	3.99	-0.095
0.500	Ge2Mg2	TlI,oS8,63	5.54	5.54	3.86	-0.104
0.538	Ge24Mg28	Ca7Sn6,oP52,62	6.70	21.43	7.34	-0.137
0.556	Ge16Mg20	Sm5Ge4,oP36,62	6.77	14.63	7.38	-0.136
0.610	Ge46Mg72	Yb36Sn23,tP118,127	10.71	10.71	20.61	-0.171
0.625	Ge12Mg20	Ba5Si3,tP32,130	6.89	6.89	13.81	-0.164
0.625	Ge18Mg30	Ca5Pb3,hP48,186	13.87	13.87	5.86	-0.165
0.625	Ge6Mg10	Cr5B3,tI32,140	8.42	8.42	8.42	-0.162
0.625	Ge6Mg10	Sr5Si3,tI32,108	8.42	8.42	8.42	-0.162
0.643	Ge10Mg18	Mg9Si5,hP28,176	7.27	7.27	12.50	-0.237
0.667	Ge1Mg2	CaF2,cF12,225	4.54	4.54	4.54	-0.277
0.667	Ge4Mg8	Co2Si-b,oP12,62	7.15	4.23	8.15	-0.224
0.750	Ge1Mg3	Cu3Au,cP4,221	4.32	4.32	4.32	-0.107
0.875	Ge1Mg7	CuPt7,cF32,225	6.27	6.27	6.27	-0.023

Table 4: Same as Tab. 1 for Mg-Ge.

Mg content	composition	structure type	a[Å]	b[Å]	c[Å]	E_f [eV/atom]
0.200	Mg2Sn8	SrSn4,oS20,63	8.73	8.73	6.50	-0.000
0.250	Mg1Sn3	Cu3Au,cP4,221	4.72	4.72	4.72	-0.021
0.250	Mg1Sn3	SrPb3,tP4,123	4.69	4.69	4.74	-0.020
0.250	Mg2Sn6	Mg3Cd,hP8,194	6.60	6.60	5.56	-0.013
0.364	Mg4Sn7	Mg4Si7,mS22,12	8.93	8.93	7.55	-0.052
0.400	Mg4Sn6	Sr2Pb3,tP10,127	8.78	8.78	3.32	-0.049
0.455	Mg5Sn6	Mg5Si6,mS22,12	9.24	9.24	7.76	-0.007
0.500	Mg1Sn1	CuAu,tP2,123	3.32	3.32	4.37	-0.115
0.500	Mg2Sn2	TlI,oS8,63	5.83	5.83	4.35	-0.056
0.556	Mg20Sn16	Sm5Ge4,oP36,62	7.37	16.60	7.43	-0.076
0.608	Mg62Sn40	Pu31Pt20,tI204,140	20.70	20.70	20.70	-0.103
0.610	Mg72Sn46	Yb36Sn23,tP118,127	11.33	11.33	22.25	-0.106
0.625	Mg10Sn6	Cr5B3,tI32,140	8.70	8.70	8.70	-0.086
0.625	Mg10Sn6	Sr5Si3,tI32,108	8.73	8.73	8.73	-0.086
0.625	Mg20Sn12	Ba5Si3,tP32,130	7.45	7.45	14.08	-0.088

0.625	Mg30Sn18	Ca5Pb3,hP48,186	15.06	15.06	5.88	-0.102
0.643	Mg18Sn10	Mg9Si5,hP28,176	7.69	7.69	13.38	-0.168
0.667	Mg2Sn1	CaF2,cF12,225	4.83	4.83	4.83	-0.178
0.667	Mg8Sn4	Co2Si-b,oP12,62	7.62	4.45	8.64	-0.148
0.750	Mg3Sn1	Cu3Au,cP4,221	4.49	4.49	4.49	-0.134
0.875	Mg7Sn1	CuPt7,cF32,225	6.39	6.39	6.39	-0.048

Table 5: Same as Tab. 1 for Mg-Sn.