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**Supporting information for article:**

**Site preference and tetragonal distortion in palladium-rich  
Heusler alloys**

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**Table S1.** Equilibrium lattice constants and total and atomic magnetic moments of L2<sub>1</sub>-type Pd<sub>2</sub>YZ alloys.

Alloy Pd <sub>2</sub> YZ	a (Å)	M <sub>t</sub> (μ <sub>B</sub> /f.u.)	M <sub>Pd-1</sub> (μ <sub>B</sub> /f.u.)	M <sub>Pd-2</sub> (μ <sub>B</sub> /f.u.)	M <sub>Y</sub> (μ <sub>B</sub> /f.u.)	M <sub>Z</sub> (μ <sub>B</sub> )
Pd <sub>2</sub> CoB	5.76	1.7708	0.05	0.05	1.71	-0.04
Pd <sub>2</sub> CoAl	6.06	1.78577	0.03	0.03	1.75	-0.03
Pd <sub>2</sub> CoGa	6.07	1.81965	0.03	0.03	1.76	-0.03
Pd <sub>2</sub> CoIn	6.31	1.89729	0.03	0.03	1.87	-0.03
Pd <sub>2</sub> CoTl	6.33	1.91239	0.04	0.04	1.84	-0.03
Pd <sub>2</sub> CoSi	5.97	1.64793	0.03	0.03	1.6	-0.02
Pd <sub>2</sub> CoGe	6.05	1.73235	0.04	0.04	1.66	-0.01
Pd <sub>2</sub> CoSn	6.29	1.79537	0.03	0.03	1.75	-0.02
Pd <sub>2</sub> CoPb	6.38	1.86218	0.05	0.05	1.78	-0.02
Pd <sub>2</sub> CoP	5.98	1.90466	0.1	0.1	1.7	0
Pd <sub>2</sub> CoAs	6.1	1.92489	0.09	0.09	1.75	-0.01
Pd <sub>2</sub> CoSb	6.29	1.84654	0.06	0.06	1.71	0.01
Pd <sub>2</sub> FeB	5.82	3.24659	0.15	0.15	2.98	-0.04
Pd <sub>2</sub> FeAl	6.1	3.23594	0.12	0.12	3.01	-0.01
Pd <sub>2</sub> FeGa	6.11	3.06884	0.12	0.12	3.04	-0.01
Pd <sub>2</sub> FeIn	6.34	3.32204	0.11	0.11	3.12	-0.01
Pd <sub>2</sub> FeTl	6.4	3.35254	0.11	0.11	3.14	-0.01
Pd <sub>2</sub> FeSi	6.04	3.19107	0.11	0.11	2.96	0
Pd <sub>2</sub> FeGe	6.13	3.29778	0.12	0.12	3.04	0.01
Pd <sub>2</sub> FeSn	6.28	3.23755	0.1	0.1	3.04	0.01
Pd <sub>2</sub> FePb	6.46	3.38874	0.11	0.11	3.15	0.02
Pd <sub>2</sub> FeP	6.07	3.50098	0.19	0.19	3.08	0.04
Pd <sub>2</sub> FeAs	6.19	3.52489	0.18	0.18	3.13	0.04
Pd <sub>2</sub> FeSb	6.28	3.3978	0.14	0.14	3.05	0.07
Pd <sub>2</sub> MnB	5.82	4.02188	0.25	0.25	3.56	-0.05
Pd <sub>2</sub> MnAl	6.08 6.16 [1]	4.16817	0.23	0.23	3.69	0.02

Pd <sub>2</sub> MnGa	6.1	4.17751	0.21	0.21	3.73	0.01
Pd <sub>2</sub> MnIn	6.41 6.373 [1]	4.32227	0.17	0.17	3.96	0.02
Pd <sub>2</sub> MnTl	6.48	4.36747	0.16	0.16	4.03	0.02
Pd <sub>2</sub> MnSi	6.02	4.03623	0.18	0.18	3.66	0.01
Pd <sub>2</sub> MnGe	6.1	4.09871	0.18	0.18	3.73	0.01
Pd <sub>2</sub> MnSn	6.33 6.38 [1]	4.16845	0.15	0.15	3.86	0.02
Pd <sub>2</sub> MnPb	6.54	4.37833	0.15	0.15	4.05	0.03
Pd <sub>2</sub> MnP	6.04	4.18373	0.19	0.19	3.79	0.01
Pd <sub>2</sub> MnAs	6.27	4.26885	0.17	0.17	3.94	0
Pd <sub>2</sub> MnSb	6.33	4.31233	0.17	0.17	3.91	0.06

## References

- [1] Webster, P. J., & Tebble, R. S. (1968). Magnetic and chemical order in Pd<sub>2</sub>MnAl in relation to order in the Heusler alloys Pd<sub>2</sub>MnIn, Pd<sub>2</sub>MnSn, and Pd<sub>2</sub>MnSb. *Journal of Applied Physics*, 39(2), 471-473.

**Table S2.** Equilibrium lattice constants and total and atomic magnetic moments of XA-type Pd<sub>2</sub>YZ alloys.

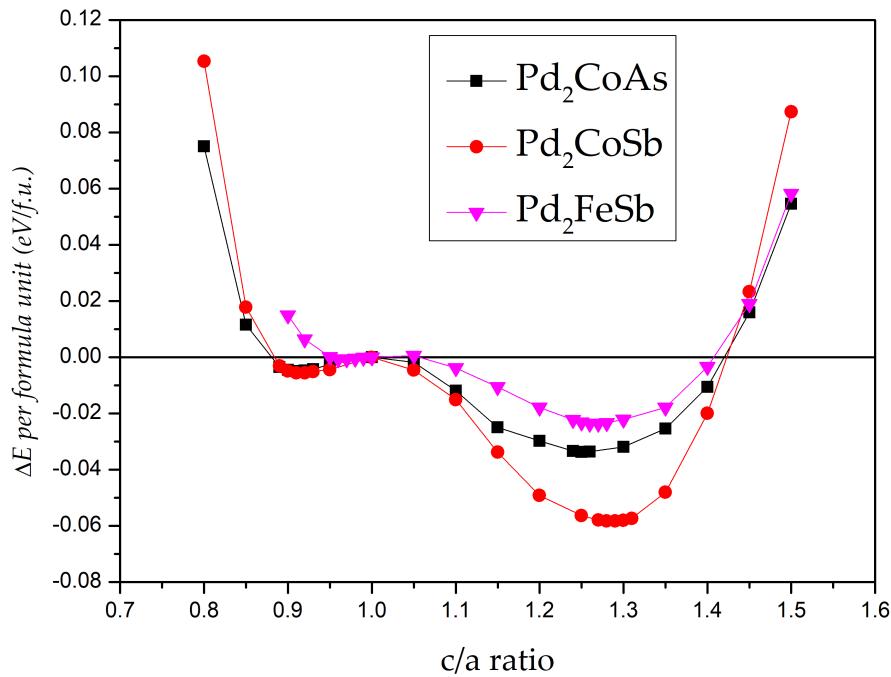
<b>Alloy</b>	<b>a (Å)</b>	<b>M<sub>t</sub></b> (μ <sub>B</sub> /f.u.)	<b>M<sub>Pd-1</sub></b> (μ <sub>B</sub> /f.u.)	<b>M<sub>Pd-2</sub></b> (μ <sub>B</sub> /f.u.)	<b>M<sub>Y</sub></b> (μ <sub>B</sub> /f.u.)	<b>M<sub>Z</sub> (μ<sub>B</sub>)</b>
<b>Pd<sub>2</sub>YZ</b>						
Pd <sub>2</sub> CoB	5.81	1.80618	0.08	0.18	1.61	-0.07
Pd <sub>2</sub> CoAl	6.08	1.65988	0.05	0.15	1.52	-0.05
Pd <sub>2</sub> CoGa	6.07	1.72374	0.05	0.16	1.556	-0.05
Pd <sub>2</sub> CoIn	6.41	1.87099	0.04	0.14	1.74	-0.05
Pd <sub>2</sub> CoTl	6.33	1.81253	0.04	0.14	1.66	-0.04
Pd <sub>2</sub> CoSi	5.98	1.30642	0.02	0.08	1.25	-0.05
Pd <sub>2</sub> CoGe	6.06	1.42584	0.02	0.09	1.35	-0.04
Pd <sub>2</sub> CoSn	6.28	1.45054	0.02	0.07	1.4	-0.04
Pd <sub>2</sub> CoPb	6.36	1.50025	0.02	0.08	1.44	-0.04
Pd <sub>2</sub> CoP	5.99	1.6766	0.05	0.13	1.5	0
Pd <sub>2</sub> CoAs	6.1	1.77839	0.06	0.14	1.58	0
Pd <sub>2</sub> CoSb	6.27	1.21614	0	0.03	1.21	-0.03
Pd <sub>2</sub> FeB	5.8	2.71517	0.04	0.21	2.57	-0.11
Pd <sub>2</sub> FeAl	6.1	2.81636	0.2	0.22	2.61	-0.03
Pd <sub>2</sub> FeGa	6.11	2.88366	0.03	0.2	2.69	-0.04
Pd <sub>2</sub> FeIn	6.32	2.99234	0.03	0.18	2.81	-0.03
Pd <sub>2</sub> FeTl	6.38	3.08977	0.04	0.18	2.89	-0.02
Pd <sub>2</sub> FeSi	6.03	2.74583	0.06	0.22	2.52	-0.04
Pd <sub>2</sub> FeGe	6.05	2.82792	0.06	0.22	2.57	-0.02
Pd <sub>2</sub> FeSn	6.27	2.88739	0.05	0.2	2.65	-0.01
Pd <sub>2</sub> FePb	6.43	3.0569	0.05	0.2	2.81	-0.01
Pd <sub>2</sub> FeP	5.96	2.93078	0.1	0.23	2.6	0
Pd <sub>2</sub> FeAs	6.07	2.99786	0.1	0.22	2.67	0
Pd <sub>2</sub> FeSb	6.26	2.74105	0.05	0.18	2.53	-0.01
Pd <sub>2</sub> MnB	5.94	3.63052	0.06	0.19	3.48	-0.1
Pd <sub>2</sub> MnAl	6.2	3.85374	0.05	0.2	3.56	0.04
Pd <sub>2</sub> MnGa	6.09	3.7741	0.06	0.2	3.48	0.03

Pd <sub>2</sub> MnIn	6.3	3.95839	0.06	0.18	3.66	0.06
Pd <sub>2</sub> MnTl	6.36	4.00153	0.04	0.17	3.73	0.04
Pd <sub>2</sub> MnSi	6.01	3.31459	0.05	0.16	3.1	0
Pd <sub>2</sub> MnGe	6.09	3.52838	0.05	0.15	3.31	0.01
Pd <sub>2</sub> MnSn	6.31	3.72078	0.05	0.14	3.49	0.04
Pd <sub>2</sub> MnPb	6.53	4.06125	0.06	0.15	3.79	0.06
Pd <sub>2</sub> MnP	6	3.4776	0.04	0.18	3.25	0.01
Pd <sub>2</sub> MnAs	6.11	3.73324	0.08	0.18	3.44	0.04
Pd <sub>2</sub> MnSb	6.31	3.57519	0.02	0.15	3.36	0.04

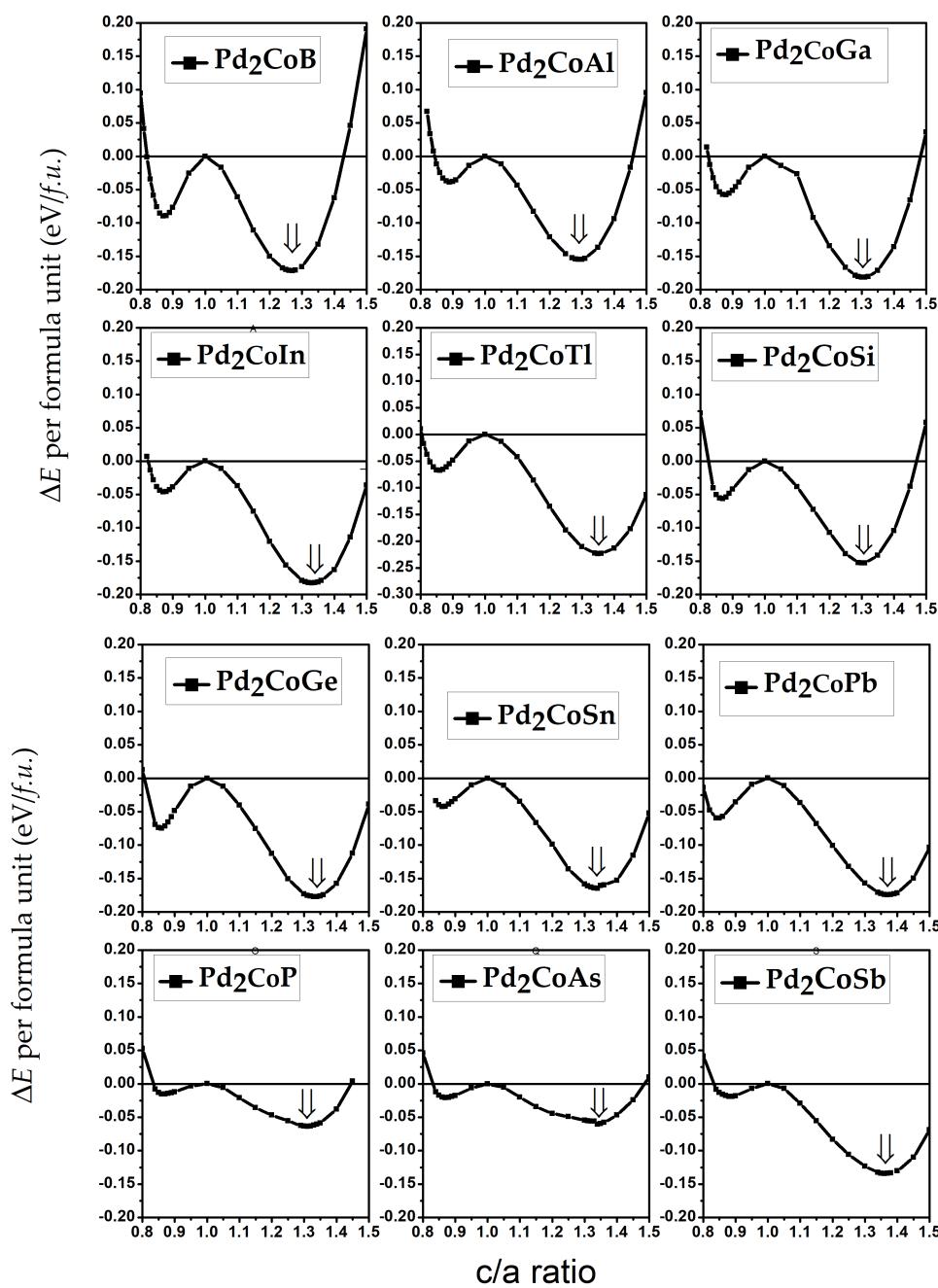
**Table S3.**  $\Delta E_M$  values, c/a ratios and total and atomic magnetic moments of L1<sub>0</sub>-type Pd<sub>2</sub>YZ in their stable phases.

Alloy Pd <sub>2</sub> YZ	$\Delta E_M$ (eV)	c/a ratio	M <sub>t</sub> ( $\mu_B$ )	M <sub>Pd</sub> ( $\mu_B$ )	M <sub>Y</sub> ( $\mu_B$ )	M <sub>Z</sub> ( $\mu_B$ )
Pd <sub>2</sub> CoB	0.17155	1.27	1.7708	0.05	1.72	-0.04
Pd <sub>2</sub> CoAl	0.15481	1.29	1.91242	0.13	1.69	-0.04
Pd <sub>2</sub> CoGa	0.18153	1.3	1.97763	0.14	1.74	-0.04
Pd <sub>2</sub> CoIn	0.18286	1.33	2.01185	0.12	1.8	-0.04
Pd <sub>2</sub> CoTl	0.22354	1.35	2.0397	0.13	1.81	-0.03
Pd <sub>2</sub> CoSi	0.15304	1.3	1.61873	0.06	1.54	-0.03
Pd <sub>2</sub> CoGe	0.17714	1.33	1.75641	0.08	1.62	-0.02
Pd <sub>2</sub> CoSn	0.16479	1.34	1.71536	0.05	1.65	-0.03
Pd <sub>2</sub> CoPb	0.17433	1.37	1.83629	0.07	1.71	-0.02
Pd <sub>2</sub> CoP	0.06372	1.31	2.28633	0.24	1.75	0.06
Pd <sub>2</sub> CoAs	0.06072	1.34	2.26212	0.22	1.77	0.05
Pd <sub>2</sub> CoSb	0.13434	1.36	1.87862	0.12	1.63	0.01
Pd <sub>2</sub> FeB	0.09957	1.29	3.30537	0.22	2.95	-0.08
Pd <sub>2</sub> FeAl	0.03091	1.26	3.1361	0.14	2.88	-0.03
Pd <sub>2</sub> FeGa	0.06703	1.3	3.23349	0.16	2.94	-0.03
Pd <sub>2</sub> FeIn	0.04623	1.31	3.2314	0.13	3.01	-0.03
Pd <sub>2</sub> FeTl	0.09271	1.34	3.30538	0.14	3.05	-0.03
Pd <sub>2</sub> FeSi	0.04330	0.85	3.15002	0.14	2.89	-0.02
Pd <sub>2</sub> FeGe	0.06845	0.84	3.24553	0.15	2.97	-0.01
Pd <sub>2</sub> FeSn	0.05061	1.27	3.11084	0.09	2.94	-0.01
Pd <sub>2</sub> FePb	0.04005	0.83	3.30681	0.12	3.07	-0.01
Pd <sub>2</sub> FeP	0.103511	1.38	3.62641	0.3	2.96	0.06
Pd <sub>2</sub> FeAs	0.08326	1.4	3.60818	0.28	2.99	0.05
Pd <sub>2</sub> FeSb	0.08487	1.38	3.274	0.2	2.83	0.04
Pd <sub>2</sub> MnB	0.10918	1.28	4.03993	0.3	3.5	-0.05
Pd <sub>2</sub> MnGa	0.04288	1.29	4.13138	0.24	3.64	0.01
Pd <sub>2</sub> MnTl	0.02044	1.31	4.35991	0.19	3.94	0.03

Pd <sub>2</sub> MnP	0.07809	1.35	4.08563	0.21	3.67	0
Pd <sub>2</sub> MnAs	0.01594	1.24	4.11632	0.14	3.87	-0.03
Pd <sub>2</sub> MnSb	0.02028	1.25	4.1728	0.16	3.81	0.04

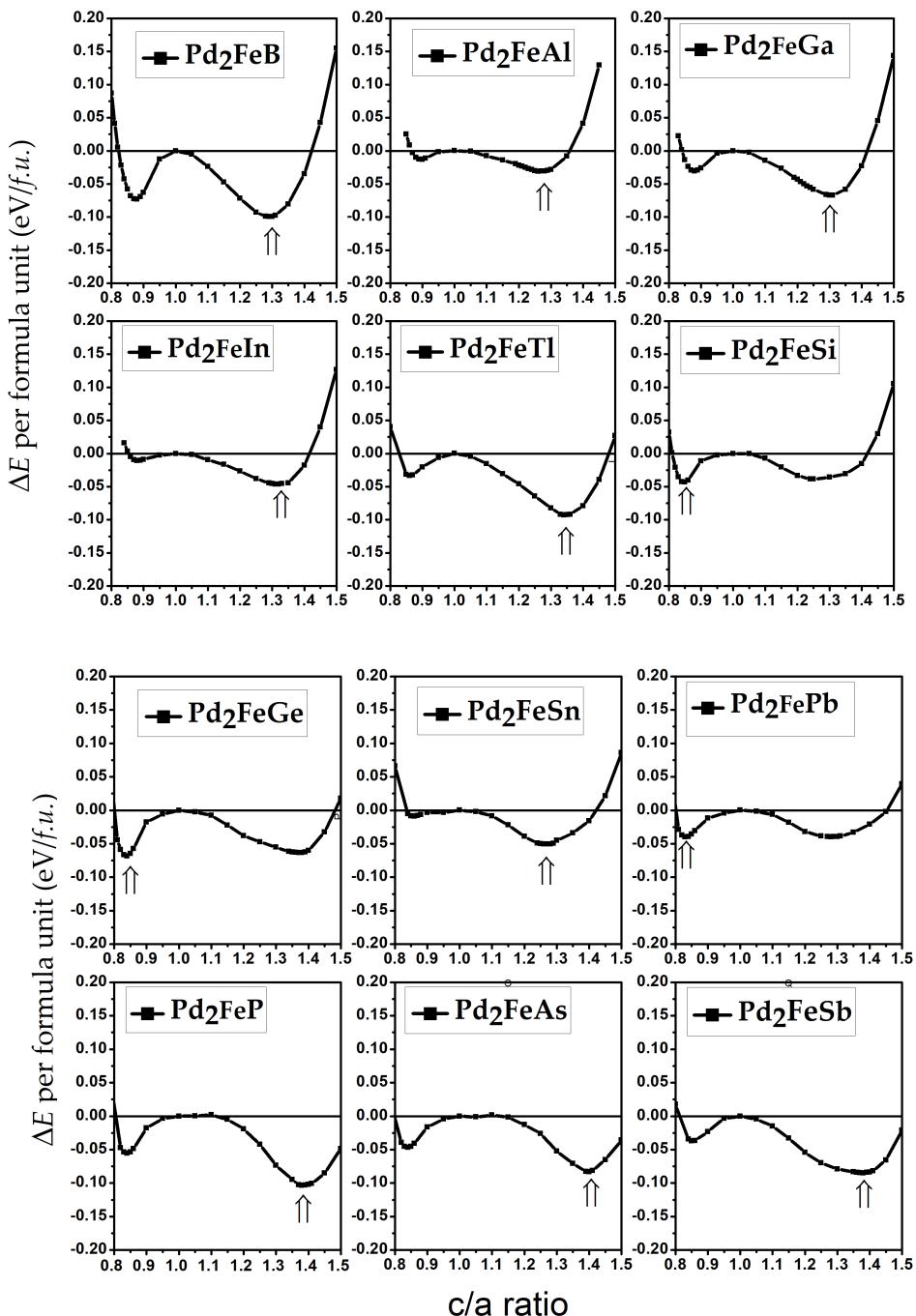


**Supplementary Figure S1** Total energies as functions of the c/a ratio for XA-type full-Heusler alloys Pd<sub>2</sub>CoSb, Pd<sub>2</sub>CoAs, Pd<sub>2</sub>FeSb. Through regulating the c/a ratio during the tetragonal deformation, we found that the inverse tetragonal ground state is more stable than the inverse cubic state due to its lower energy.



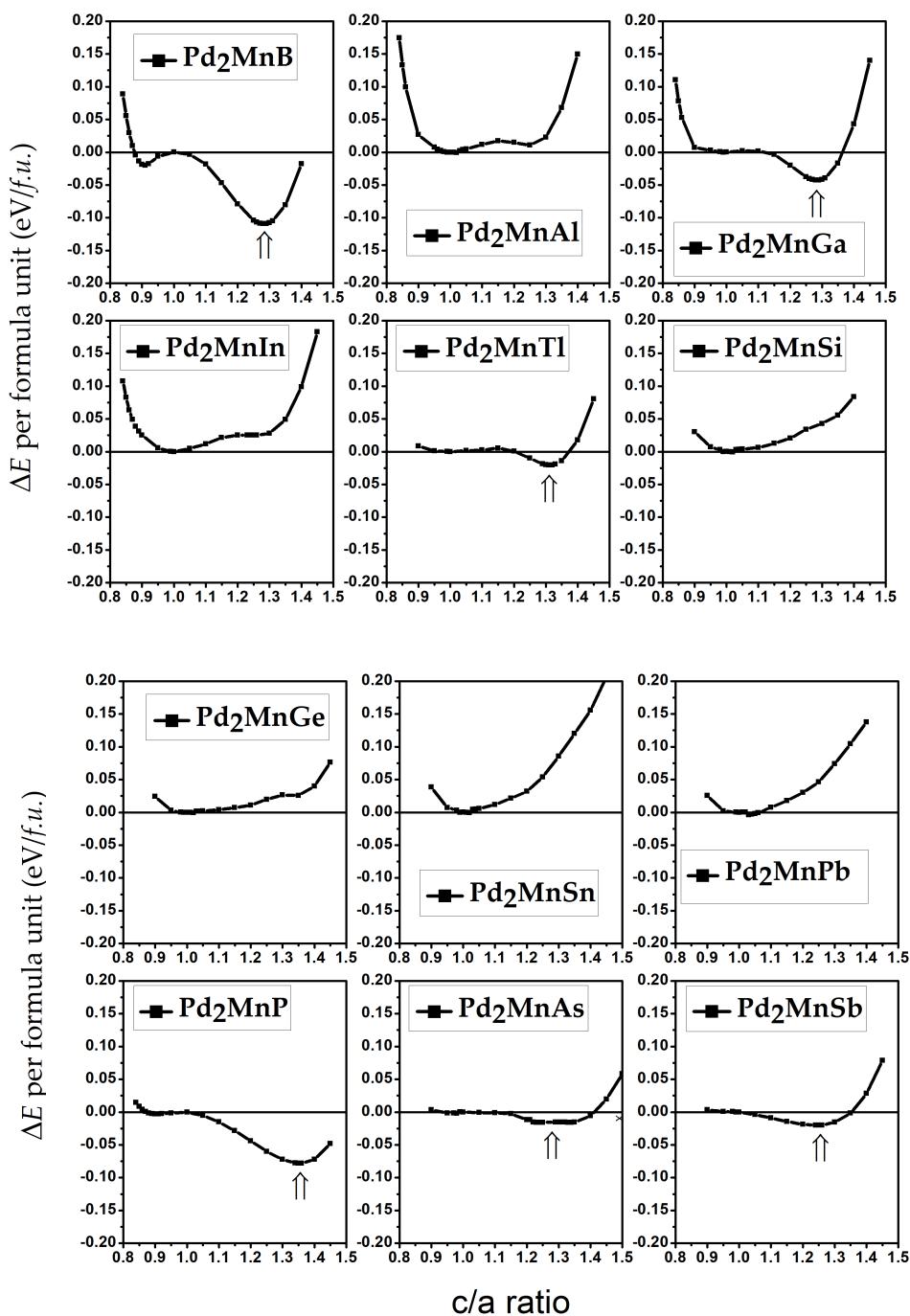
**Supplementary Figure S2** Total energies as functions of the c/a ratio for full-Heusler alloys

$\text{Pd}_2\text{CoZ}$  ( $Z = \text{B}, \text{Al}, \text{Ga}, \text{In}, \text{Tl}, \text{Si}, \text{Ge}, \text{Sn}, \text{Pb}, \text{P}, \text{As}, \text{Sb}$ ) and the corresponding  $\text{L}1_0$  phases were marked.



**Supplementary Figure S3** Total energies as functions of the c/a ratio for full-Heusler alloys

$Pd_2FeZ$  ( $Z = B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As, Sb$ ) and the corresponding  $L1_0$  phases were marked.



**Supplementary Figure S4** Total energies as functions of the c/a ratio for full-Heusler alloys

Pd<sub>2</sub>MnZ (Z = B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As, Sb) and the corresponding L<sub>1</sub><sub>0</sub> phases were marked.