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Supporting information for article:

**Effect of swap disorder on the physical properties of the
quaternary Heusler alloy PdMnTiAl: a first-principles study**

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Supplementary Materials

Swap disorder effect on the physical properties of quaternary Heusler alloy PdMnTiAl: a first-principles study

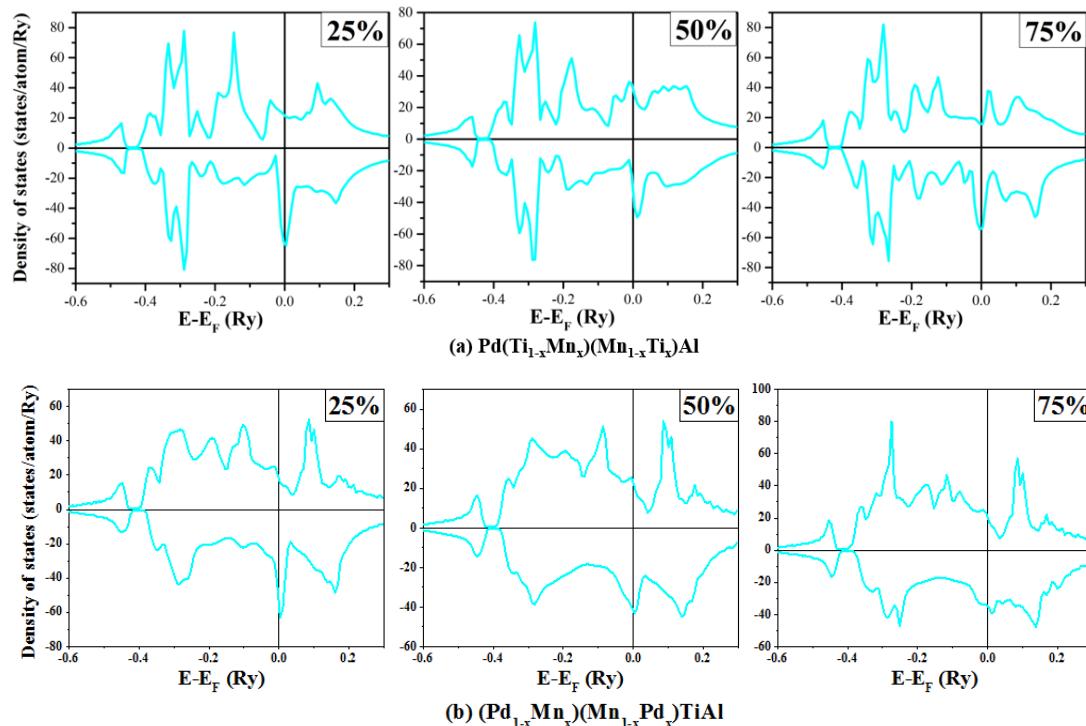
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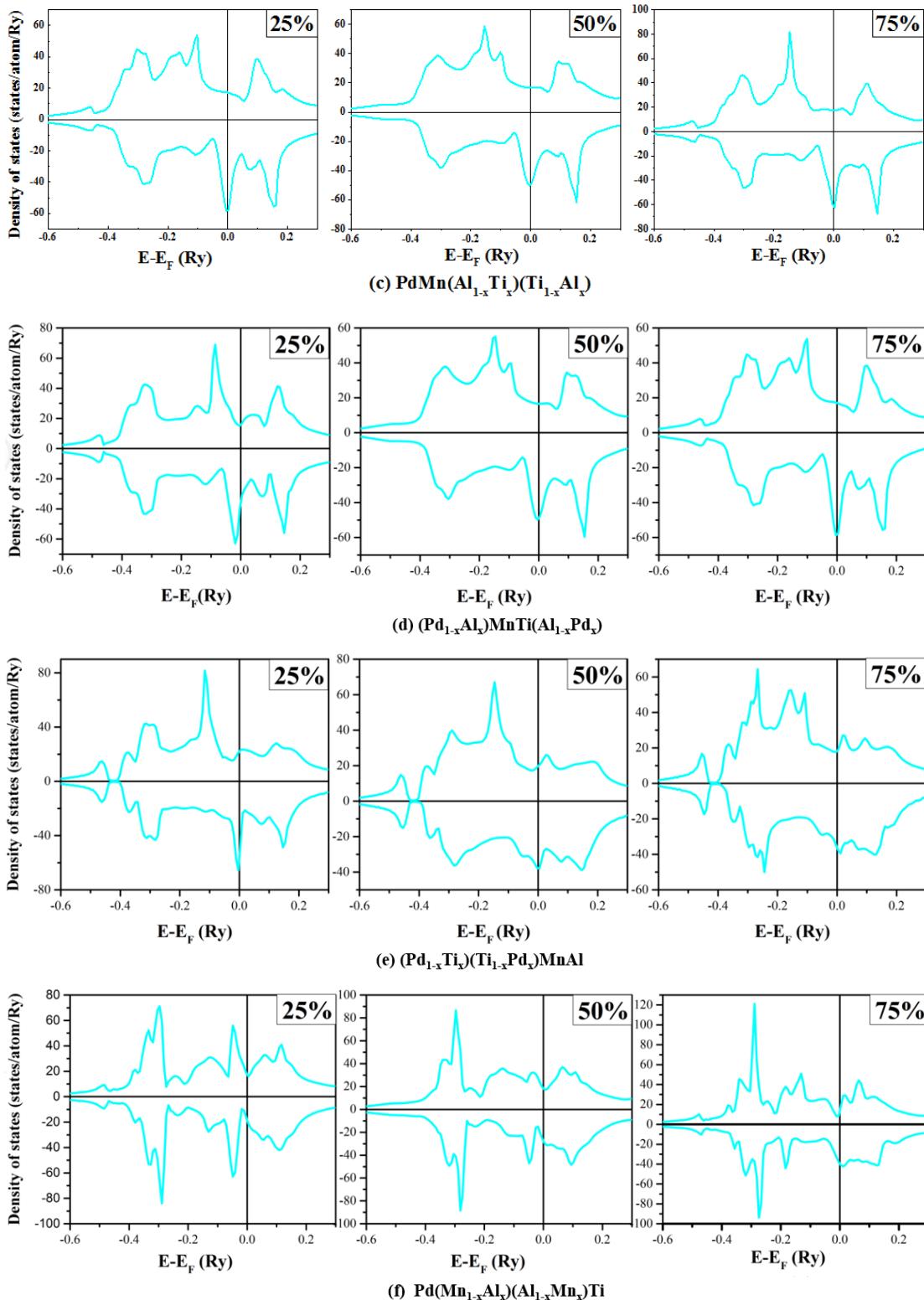
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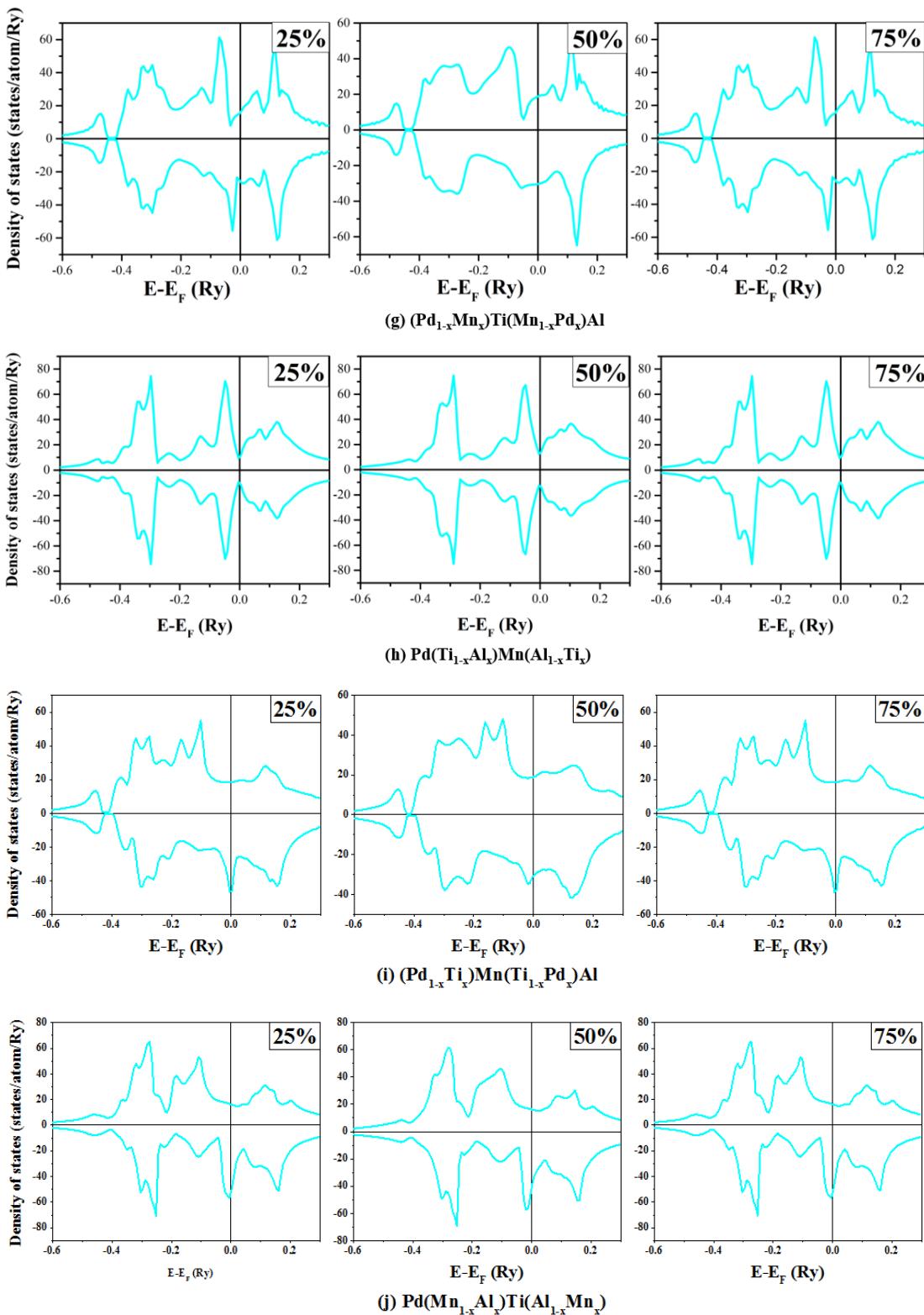
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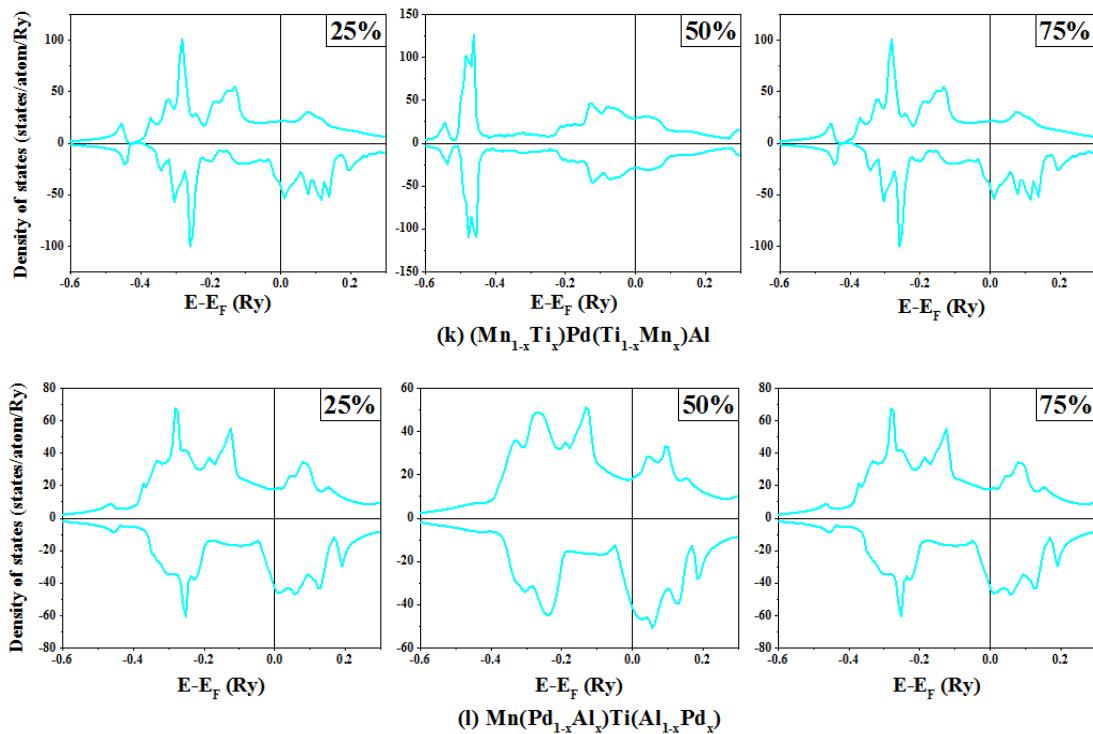


Figure S1 The density of states (DOS) of disordered structures. We present the disorder degrees of $x=25\%$, 50% and 75% with (a) Ti-Mn swap, (b) Pd-Mn swap, (c) Ti-Al swap, (d) Mn-Al swap, (e) Pd-Mn swap, (f) Ti-Al swap, (g) Pd-Mn swap, (h) Ti-Al swap, (i) Pd-Ti swap, (j) Mn-Al swap, (k) Ti-Mn swap, and (l) Pd-Al swap.

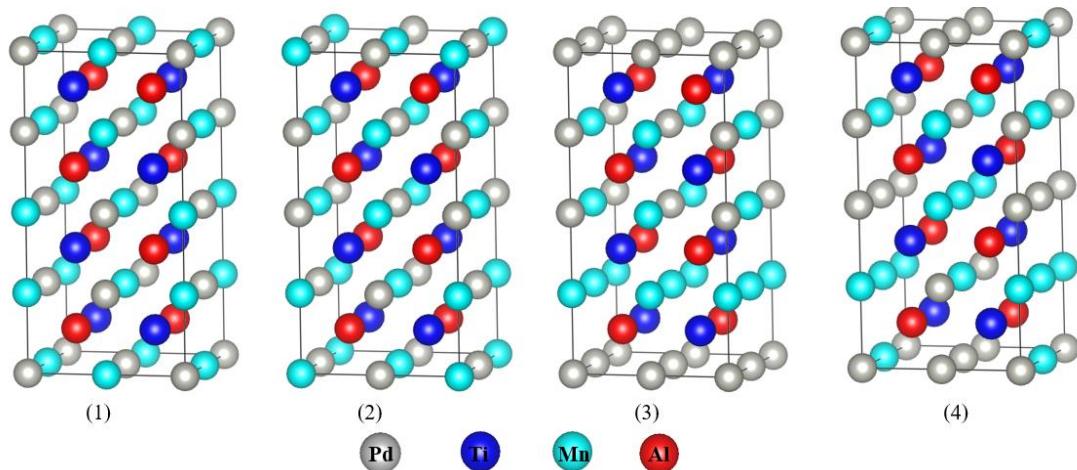


Figure S2 The different structures of 50% swap disorder in VASP supercell simulation of “disordered” structure. The grey, blue, cyan and red spheres are for Pd, Ti, Mn, and Al elements respectively.

Table S1 The results of Pd-Mn swap disorder simulations using VASP and AkaiKKR.
(The lowest energy is set as zero.)

	Swap ratio	Total energy	Magnetic moment
VASP	0%	0eV	0 μ_B
	25%	-0.377eV	0.440 μ_B
	50%(1)	-0.080eV	0.120 μ_B
	50%(2)	-0.043eV	0.108 μ_B
	50%(3)	-0.248eV	0.175 μ_B
	50%(4)	-0.228eV	0.574 μ_B
AkaiKKR	0%	0eV	0 μ_B
	25%	-0.092eV	0.803 μ_B
	50%	-0.047eV	1.132 μ_B