Supplementary Materials for

First-principles study on transport properties of quaternary CoFeZGa (Z=Ti, V, Cr, Mn, Cu, Nb) Heusler compound

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Table S1 The total energy (E_{tot}), relaxed lattice parameter (a), atom-projected magnetic moments ($M_{Y(Co,\ Fe,\ R\ and\ Ga)}$) and total magnetic moments (M_{tot}) of the three possible structural variants in non-magnetic (NM) and ferromagnetic (FM) state for quaternary Heusler alloys CoFeRGa (R= Ti, V, Cr, Mn, Cu, and Nb).

Alloys	Type	State	E_{tot} (eV)	a(Å)	Atomic magnetic moment(μ_B)				
					M_{Co}	M_{Fe}	M_R	M_{Ga}	M_{tot}
CoFeTiGa	Ⅰ	NM	-111.65258	5.81	--	--	--	--	--
	Ⅱ	FM	-107.46332	5.95	1.19	2.24	-0.38	-0.02	3.03
		NM	-104.47505	5.89	--	--	--	--	--
	Ⅲ	FM	-107.00505	5.96	1.54	2.36	-0.11	-0.00	3.79
		NM	-104.67961	5.89	--	--	--	--	--
CoFeVGa	Ⅰ	NM	-112.77346	5.73	--	--	--	--	--
	Ⅱ	FM	-110.90570	5.85	0.98	2.48	-1.21	-0.02	2.23
		NM	-107.72296	5.78	--	--	--	--	--
	Ⅲ	FM	-109.22747	5.84	1.42	2.15	-0.60	-0.01	2.96
		NM	-107.30934	5.78	--	--	--	--	--
CoFeCrGa	Ⅰ	NM	-110.29828	5.68	--	--	--	--	--
	Ⅱ	FM	-111.69683	5.79	1.06	2.63	-1.67	0.00	2.02
		NM	-108.26250	5.70	--	--	--	--	--
	Ⅲ	FM	-108.62227	5.80	1.36	2.11	0.46	-0.01	3.92
		NM	-107.35281	5.71	--	--	--	--	--
CoFeMnGa	Ⅰ	NM	-106.88443	5.66	--	--	--	--	--
	Ⅱ	FM	-109.97816	5.79	1.20	2.44	2.47	-0.09	6.02
		NM	-106.72003	5.66	--	--	--	--	--
	Ⅲ	FM	-109.39892	5.83	1.72	2.29	2.96	-0.08	6.89
		NM	-105.94877	5.66	--	--	--	--	--
CoFeCuGa	Ⅰ	FM	-87.361821	5.78	0.93	2.42	0.09	-0.08	3.36
		NM	-85.618884	5.71	--	--	--	--	--
	Ⅱ	NM	-84.931003	5.72	--	--	--	--	--
	Ⅲ	FM	-87.969075	5.78	1.34	2.24	-0.02	-0.05	3.51
		NM	-85.268646	5.72	--	--	--	--	--

CoFeNbGa	Ⅰ	NM	-117.64923	5.93	--	--	--	--	--
	Ⅱ	FM	-114.61657	6.04	1.32	2.24	-0.31	-0.02	3.23
		NM	-111.45303	5.98	--	--	--	--	--
	Ⅲ	FM	-113.67567	6.04	1.20	2.41	-0.17	-0.01	3.43
		NM	-111.45902	5.98	--	--	--	--	--

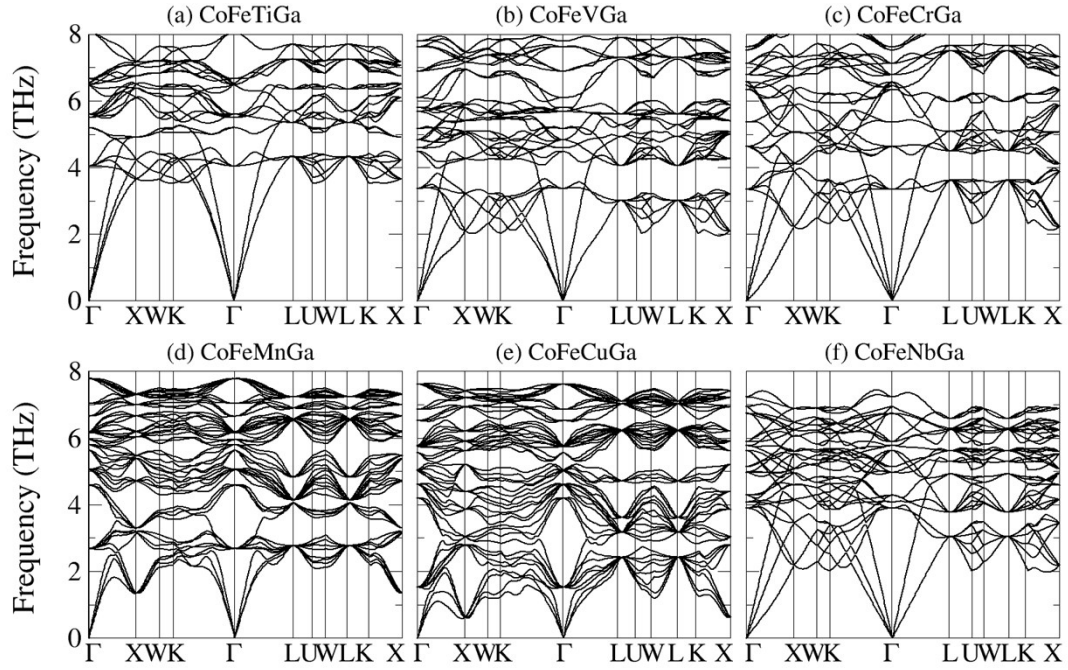

Fig. S1 The phonon spectra of CoFeRGa (R= Ti, V, Cr, Mn, Cu, and Nb) compounds in the *F-43m* phase.

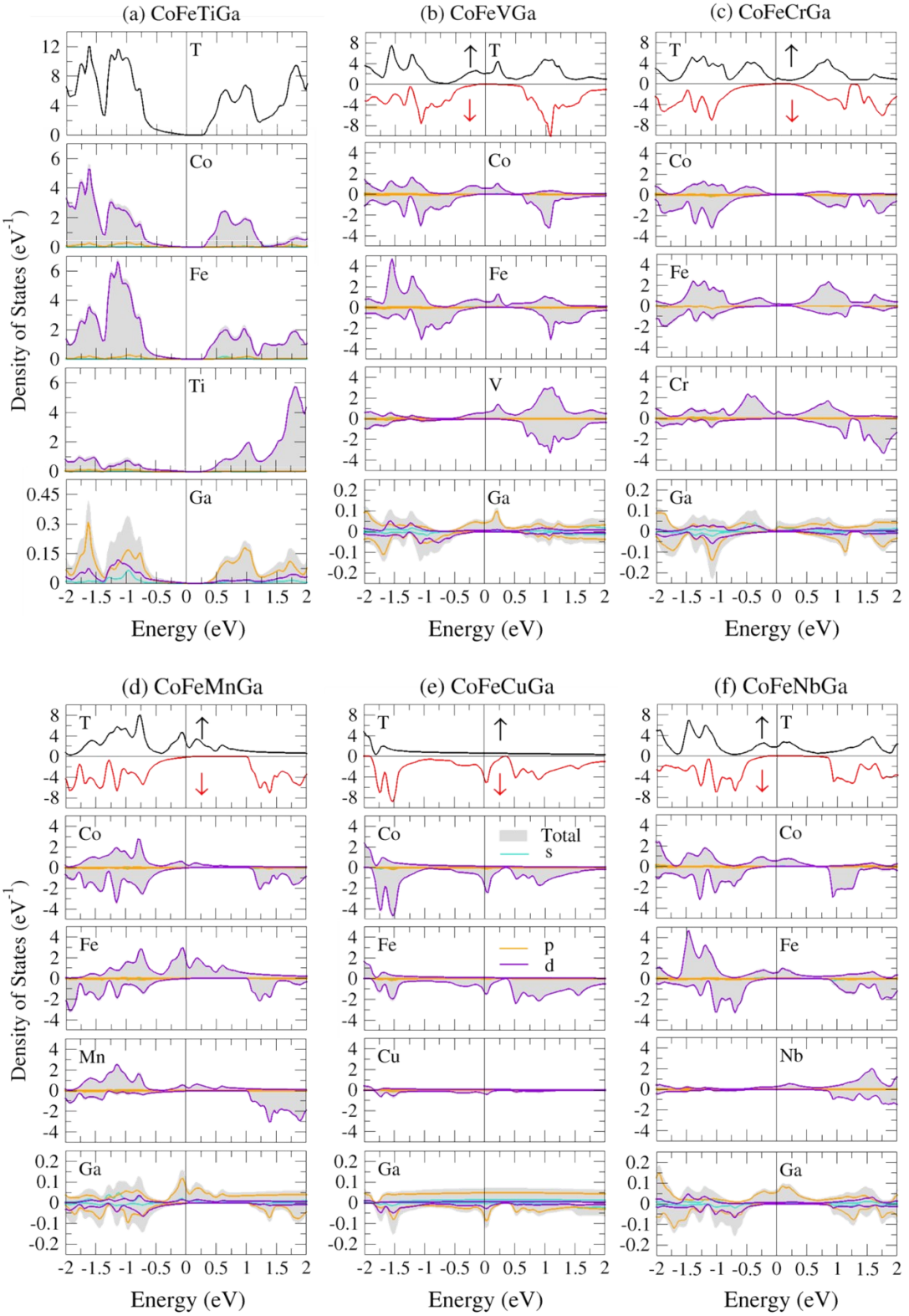

Fig. S2 The spin-dependent total density of states and partial density of states (PDOS) of Heusler alloys CoFeCrGa, CoFeMnGa, and CoFeCuGa at the ground state. The positive and negative values of the density of states are corresponded to the spin-up and spin-down channels, respectively.

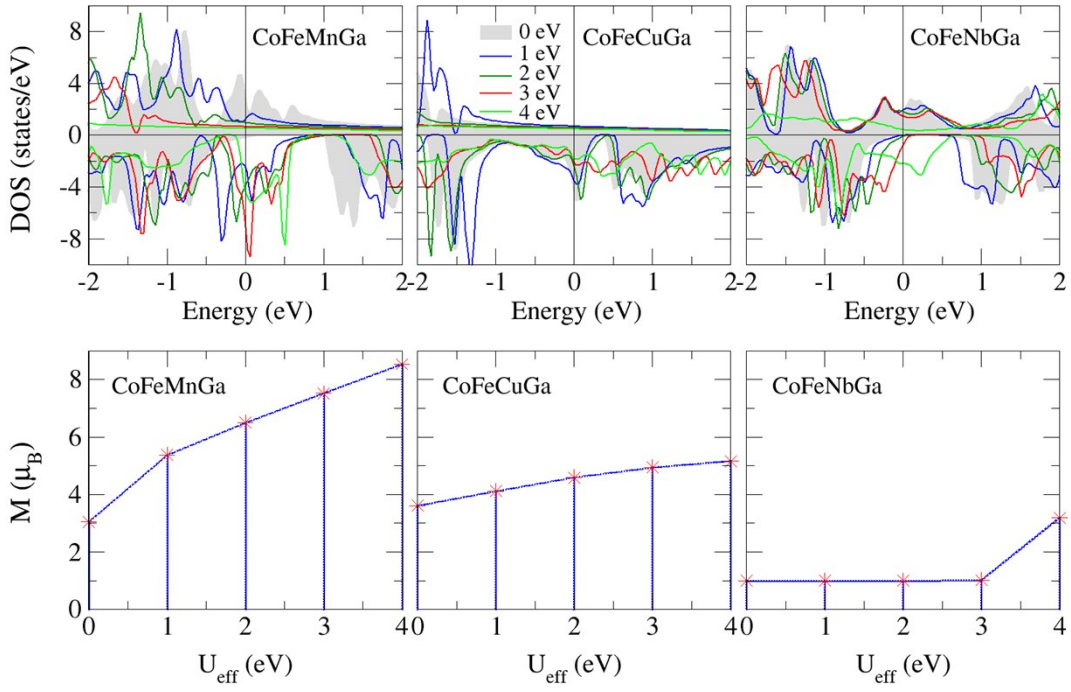

Fig. S3 The density of states and total magnetic moments under several U_{eff} (U_{eff}=1, 2, 3, and 4 eV)