

New family of NaTMGe (TM = 3d transition metals) half-Heusler compounds: the role of TM modification

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Table S1: Spin-up/spin-down band gap E_g (eV) and magnetic moments μ (T: total; I: interstitial) (μ_B) of NaTMGe half-Heusler compounds calculated with mBJ-GGA+U(mBJ-GGA).

	E_g	μ				
		T	I	Na	TM	Ge
TM = V	0.64/1.13(0.12/1.12)	2.00(2.00)	0.02(0.10)	-0.03(-0.01)	2.18(2.07)	-0.17(-0.15)
TM = Cr	M/2.01(M/1.70)	3.00(3.00)	-0.17(0.02)	-0.08(-0.04)	3.98(3.52)	-0.74(-0.50)
TM = Mn	M/1.77(M/1.53)	4.00(4.00)	-0.10(0.14)	-0.02(-0.01)	4.56(4.21)	-0.44(-0.34)
TM = Fe	M/M(M/M)	3.53(3.03)	0.15(0.10)	0.02(0.02)	3.44(3.02)	-0.07(-0.10)

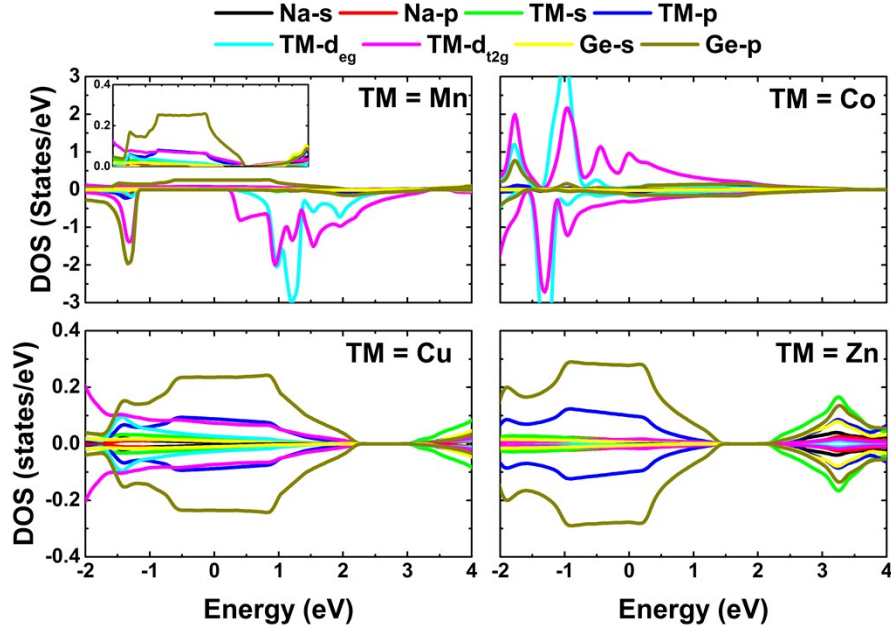


Figure S1: Projected density of states of NaMnGe, NaCoGe, NaCuGe, and NaZnGe half-Heusler compounds.

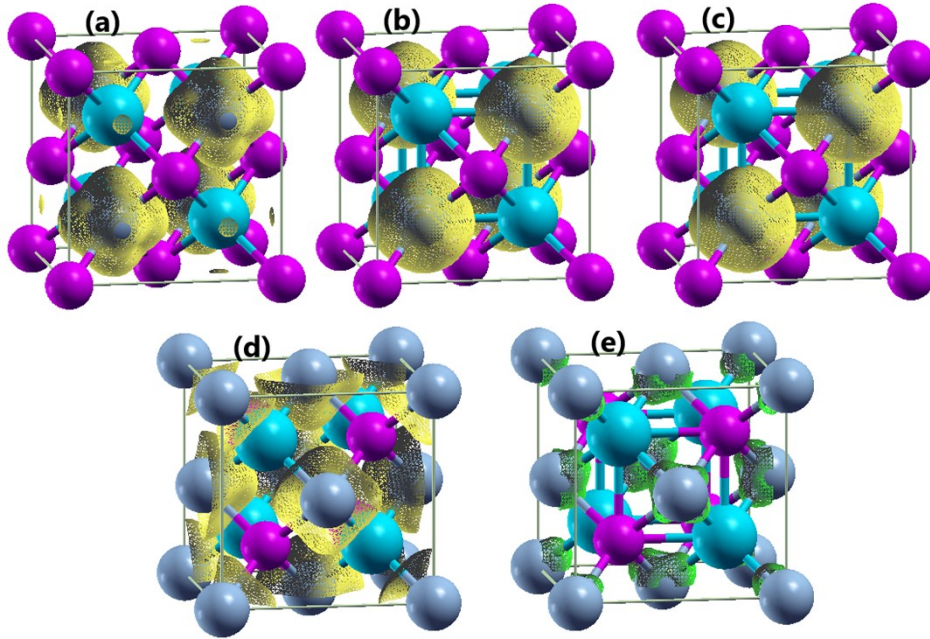


Figure S2: Spin density in NaTMGe half-Heusler compounds (Yellow isosurface: spin-up; Green isosurfa: spin-down; Isosurface value: $0.02 \text{ e}/\text{\AA}^3$) with (a) TM = V, (b) TM = Cr, (c) TM = Mn, (d) TM = Fe, and (e) TM = Co.

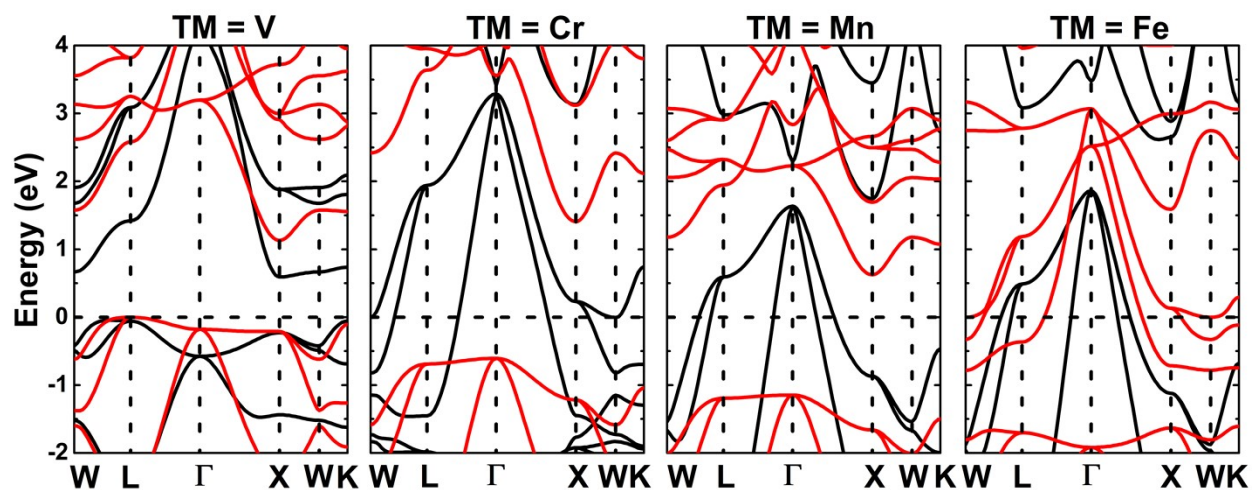


Figure S3: Electronic band structure of NaTMGe half-Heusler compounds (Black line: Spin-up; Red line: Spin-down) calculated by mBJ-GGA+U.

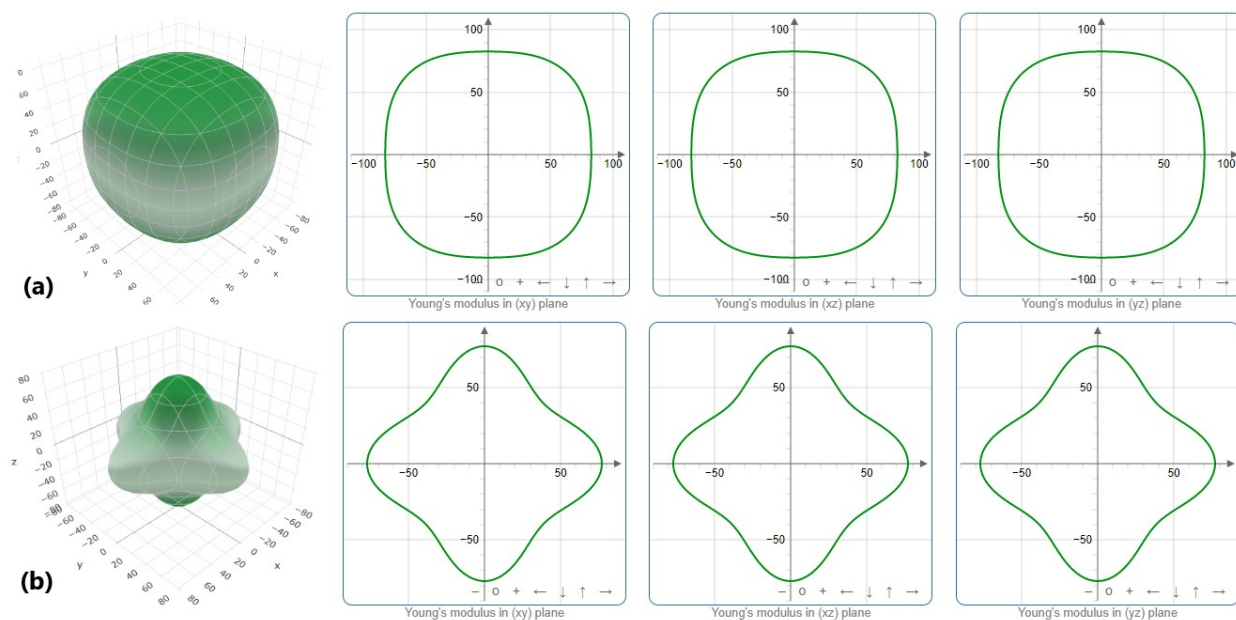


Figure S4: Directional dependence of Young modulus of (a) NaTiGe and (b) NaVGe half-Heusler compounds.

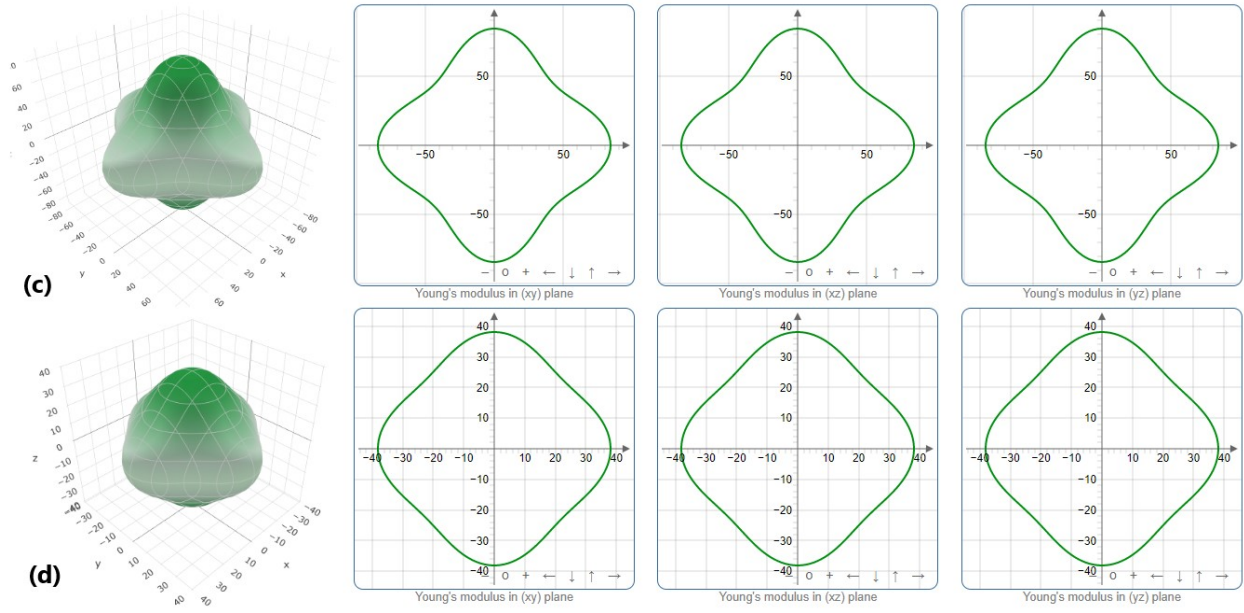


Figure S4 (Cont): (c) NaCrGe and (d) NaMnGe.

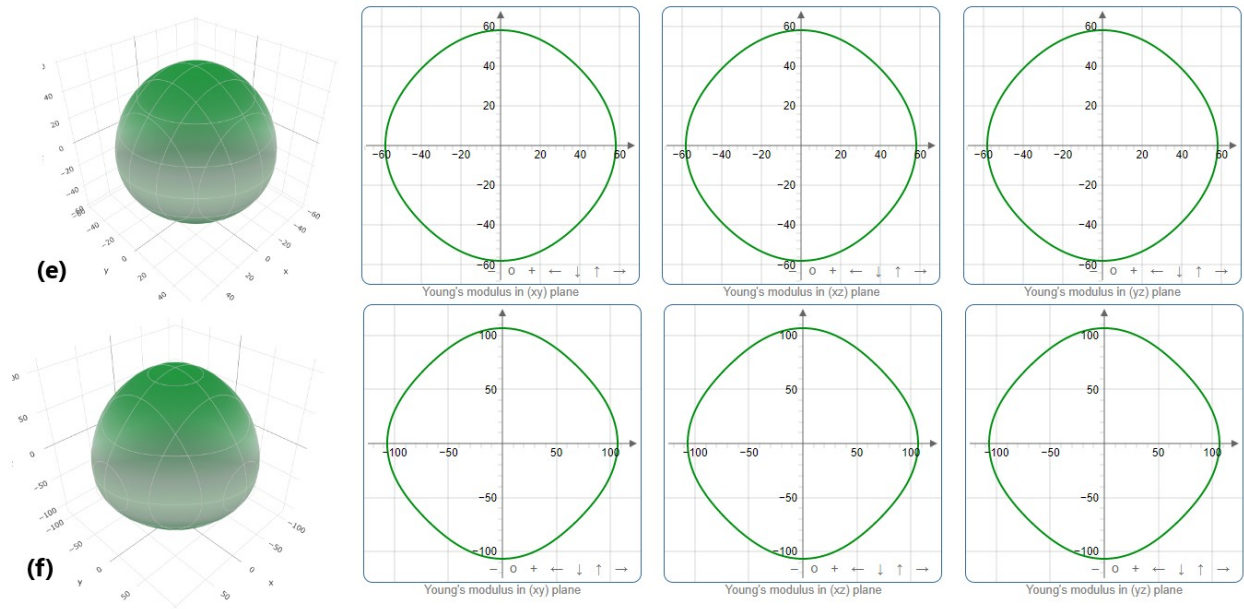


Figure S4 (Cont): (e) NaFeGe and (f) NaCoGe.

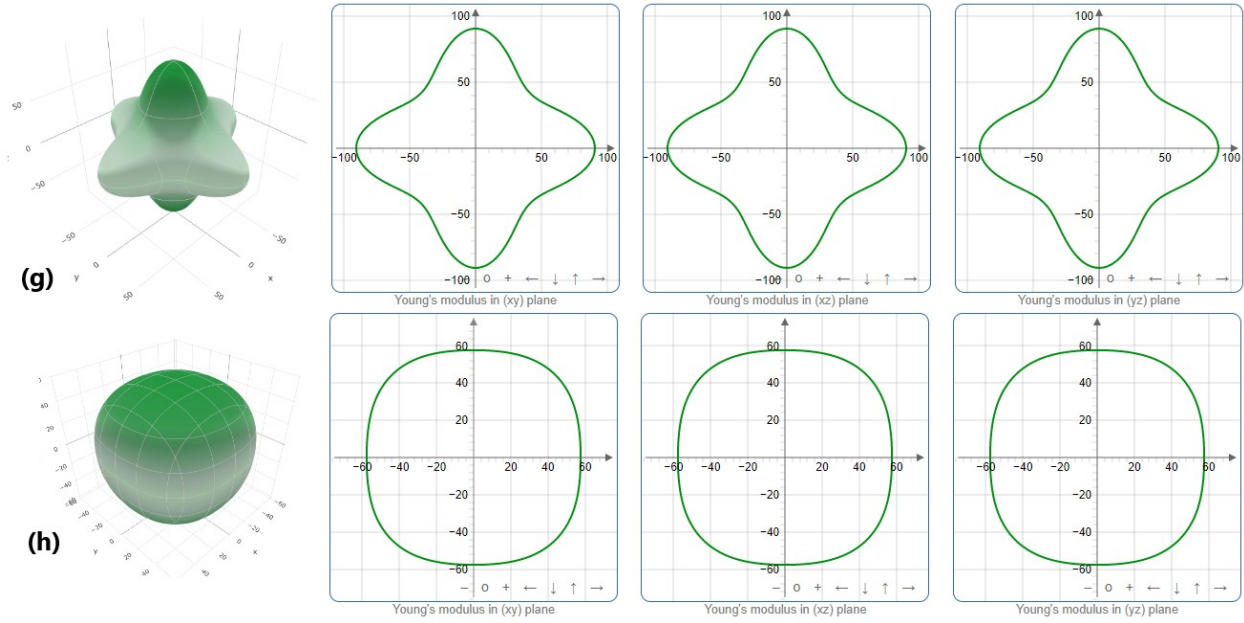


Figure S4 (Cont): (g) NaNiGe and (h) NaCuGe.