Supporting Information

Half Metal-to-Metal Transition and Superior Transport Response Holding a Very High Curie-Temperature in CoFeRuSn: Strain Regulations

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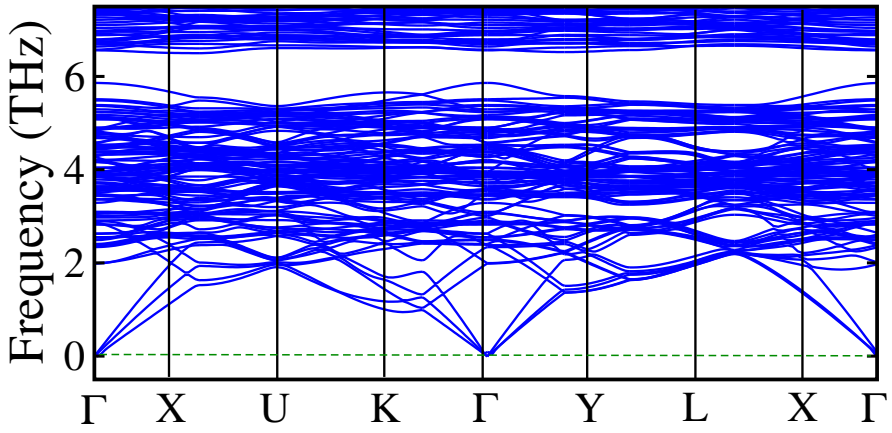

FIG. 1S: Calculated Phonon bands of the CoFeRuSn quaternary Heusler alloy.

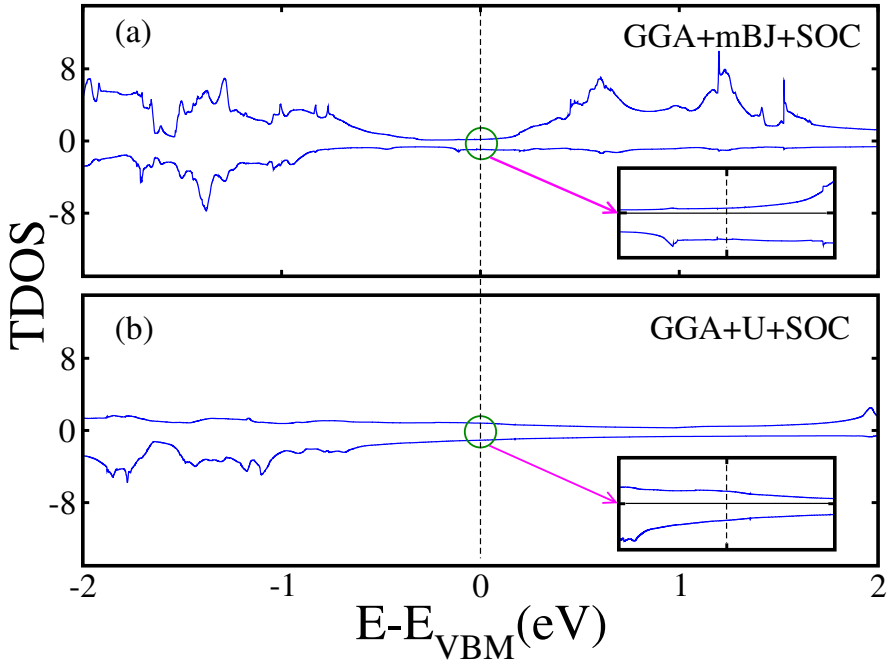

FIG. 2S: Computed (a/b) GGA+mBJ+SOC/GGA+U+SOC spin non-degenerated total density of states (TDOS) in states/eV in a stable T1 configuration for the unstrained CoFeRuSn quaternary Heusler alloy.

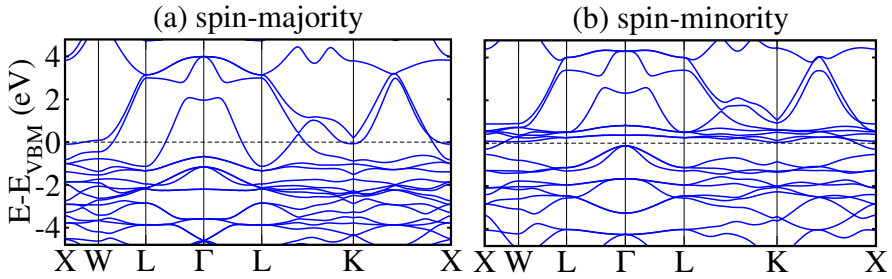

FIG. 3S: GGA calculated non-degenerated band structures for the spin-majority/spin-minority channel in (a/b) of the CoFeRuSn quaternary Heusler alloy in a stable T1 configuration.

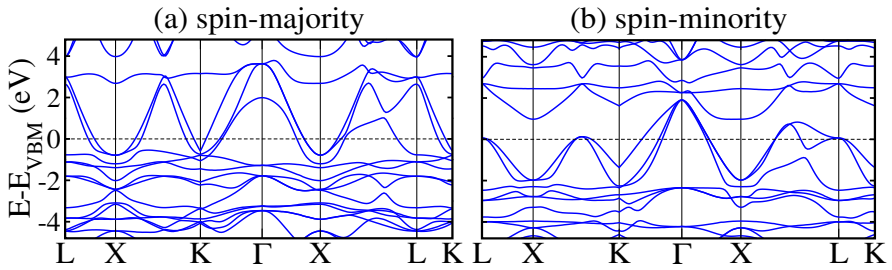

FIG. 4S: GGA+U calculated non-degenerated band structures for the spin-majority/spin-minority channel in (a/b) of the CoFeRuSn quaternary Heusler alloy in a stable T1 configuration.

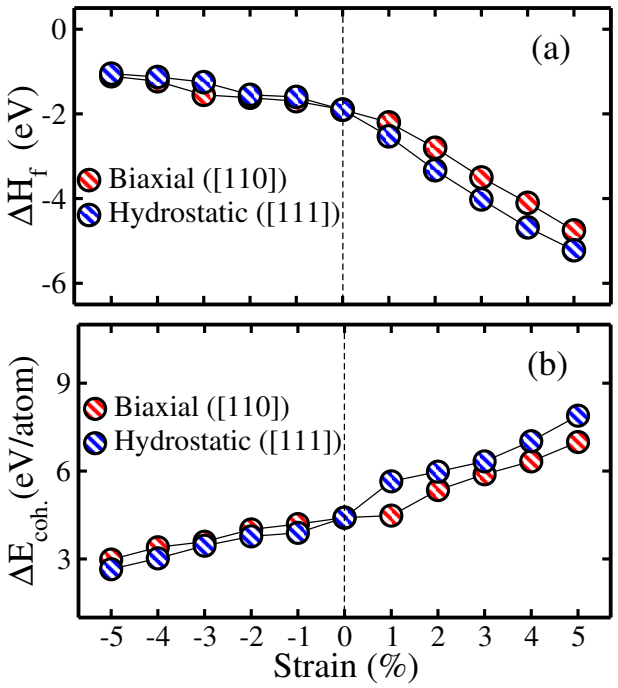

FIG. 5S: mBJ-GGA computed (a) enthalpies of formation (ΔH_f) and (b) cohesive energy ($\Delta E_{coh.}$) as a function of ± 5% biaxial ([110])/hydrostatic ([111]) strain in the CoFeRuSn quaternary Heusler alloy.

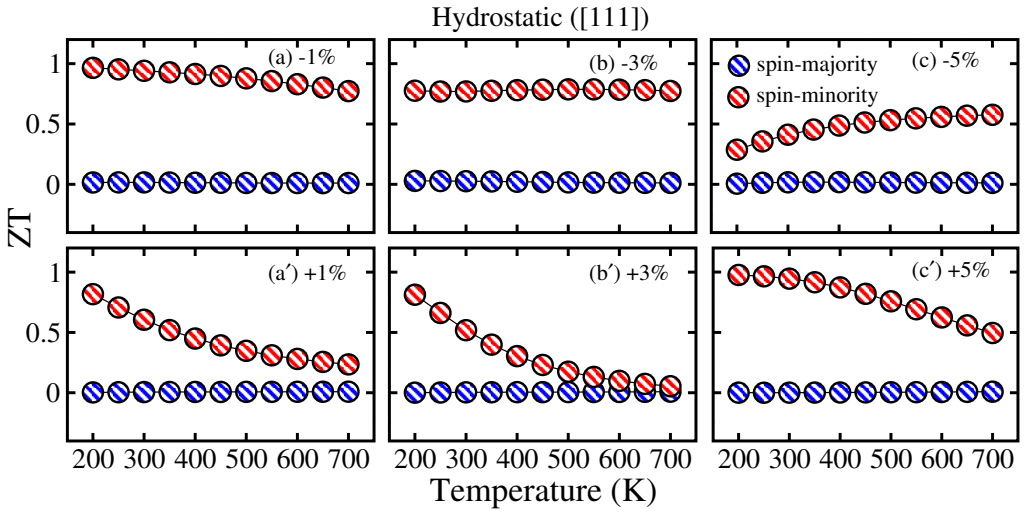

FIG. 6S: Computed figure of merit (ZT) as a function of temperature for (a/a′) −1%/+1%, (b/b′) −3%/+3% and (c/c′) −5%/+5% for hydrostatic ([111]) compressive/tensile strain in the CoFeRuSn quaternary Heusler alloy.

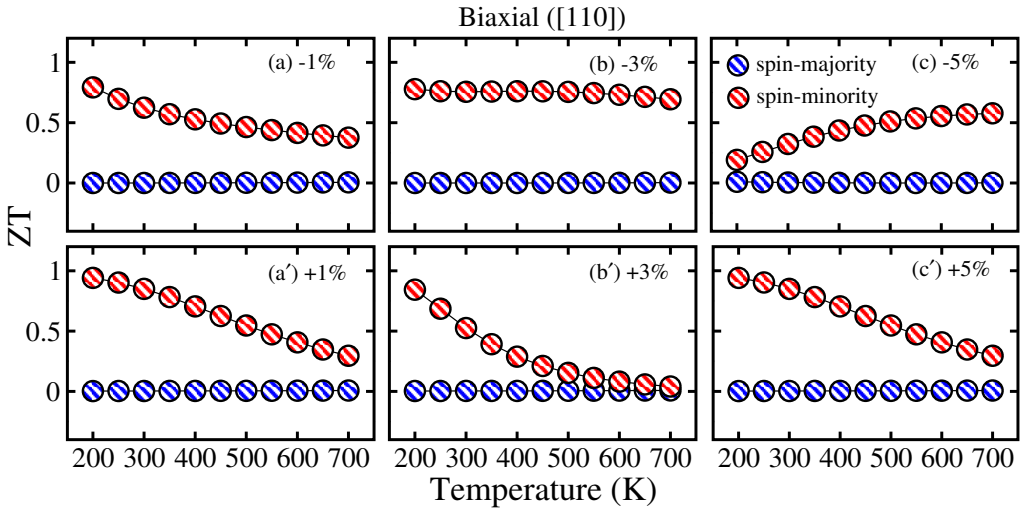

FIG. 7S: Computed figure of merit (ZT) as a function of temperature for (a/a′) −1%/+1%, (b/b′) −3%/+3% and (c/c′) −5%/+5% for biaxial ([110]) compressive/tensile strain in the CoFeRuSn quaternary Heusler alloy.