Supporting Information

Theoretical Prediction of Negative Thermal Expansion in Cubic VF_3

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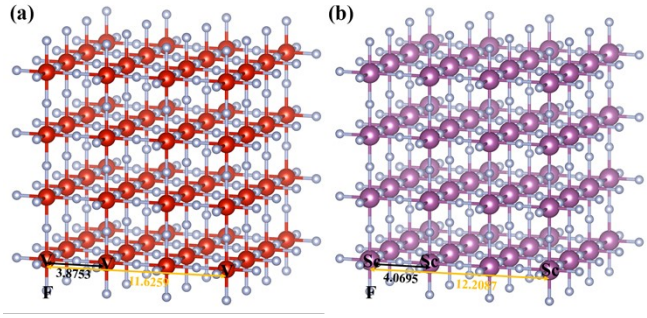

Figure S1. The 3×3×3 supercell structure of (a)VF_3 and (b)ScF_3

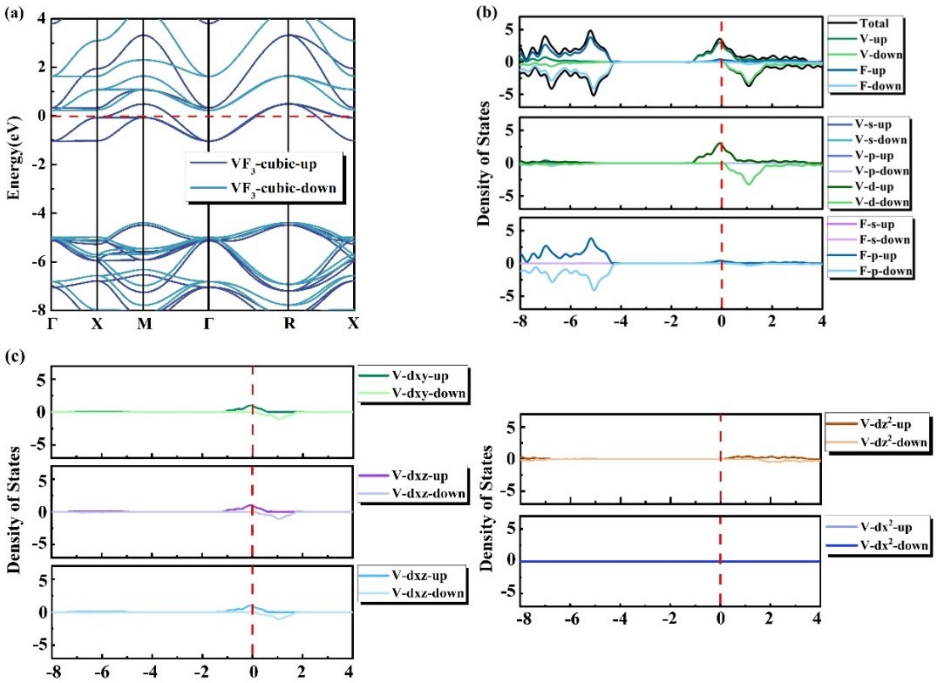

Figure S2. (a) Calculated band structure (b) density of states of cubic VF_3.

(c) d-orbitals of V atom. Red dashed line indicates Fermi level.

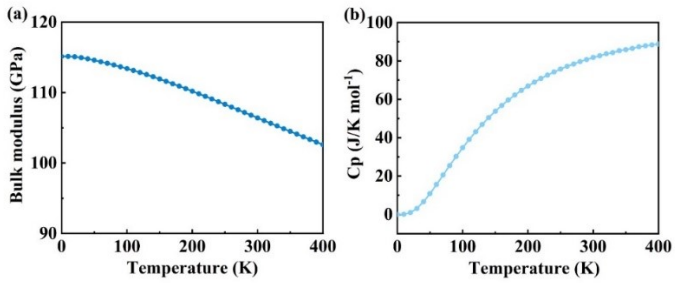

Figure S3. Calculated thermodynamic properties of VF_3 versus temperature: (a) bulk modulus (*B*);

(b) heat capacities (C_p).

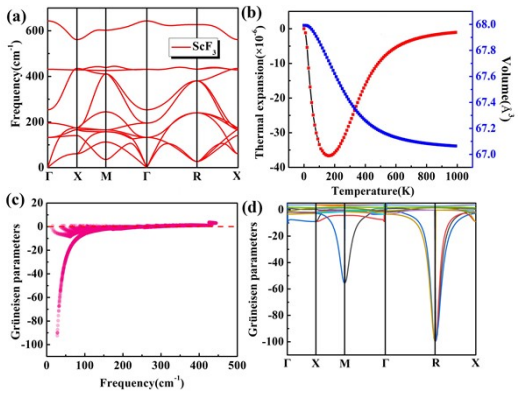

Figure S4. (a) Phonon dispersion(b) NTE and unit volume versus temperature (c) Phonon mode Grüneisen parameter (d) Grüneisen parameter along high symmetry direction of cubic ScF_3

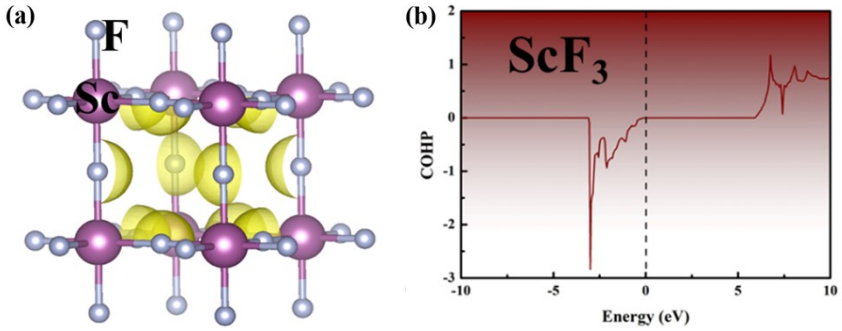

Figure S5. (a) Electron localization function (ELF) (isosurface value:0.6 $born^{-3}$) of ScF_3, Red, brown atoms denote V and F atoms, respectively. (b) The calculated COHP of ScF_3.

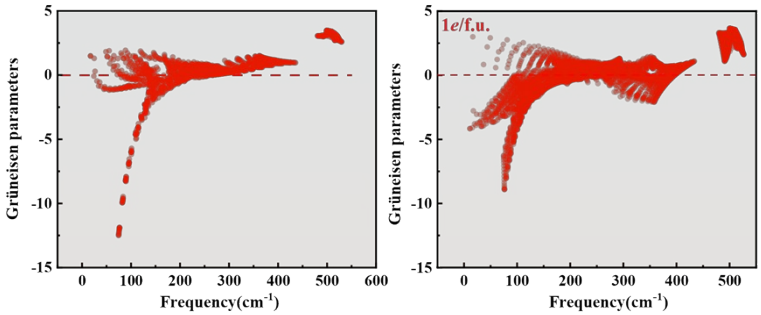

Figure S6. Calculated mode Grüneisen parameters of cubic supercell $V_{27}F_{81}$ with 0 e and 1 e, respectively. (1e/f.u.: adding one electron into the supercell $V_{27}F_{81}$)

Table S1. Elastic properties of cubic VF_3.

	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	G (GPa)	E (GPa)
VF_3	299.26	35.29	25.73	123.28	53.09	139.27

Table S2 Calculated Grüneisen parameters(γ_i) of cubic VF_3 at the M (0.5, 0.5, 0) and R (0.5, 0.5, 0.5) points, and compared with isostructural ScF_3 and ReO_3.

Compounds	M (0.5, 0.5, 0) Frequency (cm^{-1})	γ_i	R (0.5, 0.5, 0.5) Frequency (cm^{-1})	γ_i	Maximum NTE ($\times10^{-6}$ K^{-1})	References
VF_3	72.48	-12.53	74.47	-11.82	-6.41 (80 K)	This work
ScF_3	34.85	-57.72	34.65	-98.81	-32.72(160 K)	This work
	34.92	-80.46	33.72	-85.50	-24.54 (90 K)	Comp.Mater.Sci. 2015,107,157-162.
ReO_3	73.99	-16.39	88.19	-13.39	-1.55 (80 K)	