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Ab initio study of the piezomagnetic effect and mechanocaloric effects in Mn-antiperovskites

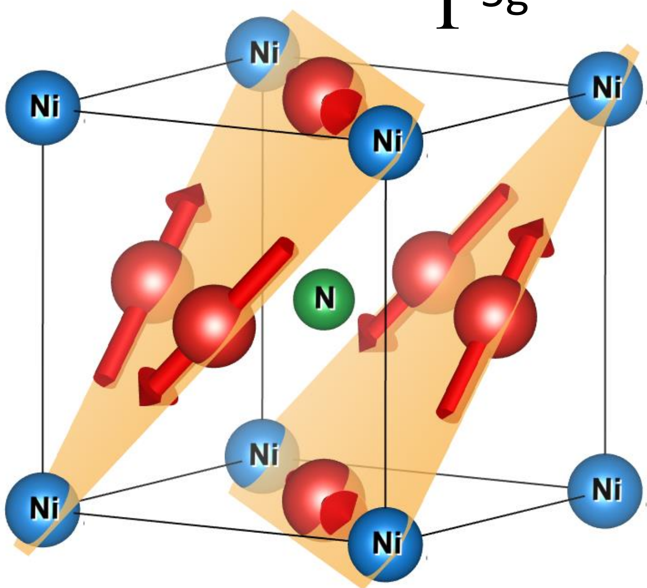
Jan Zemen, Zsolt Gercsi, Karl G. Sandeman

DDMC 2015

DRREAM

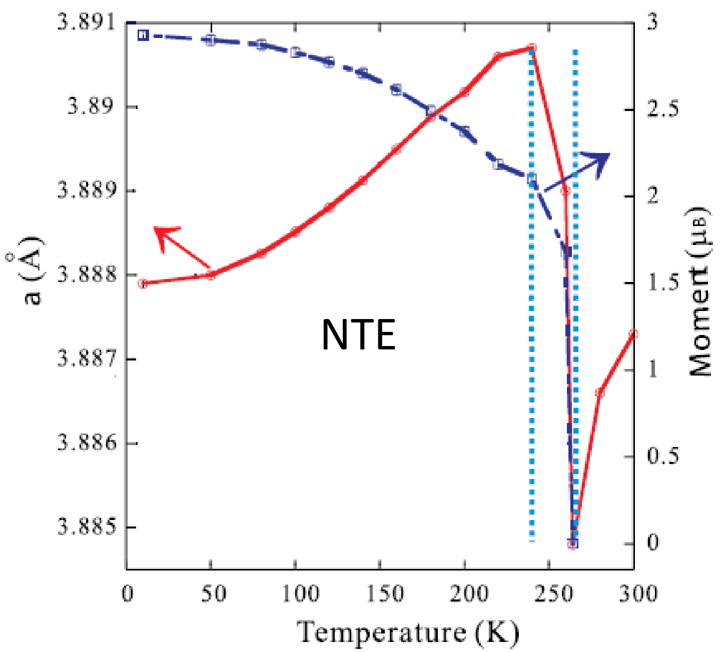
Drastically Reduced Use of Rare Earths in Applications of Magnetocalorics

Γ^{5g}

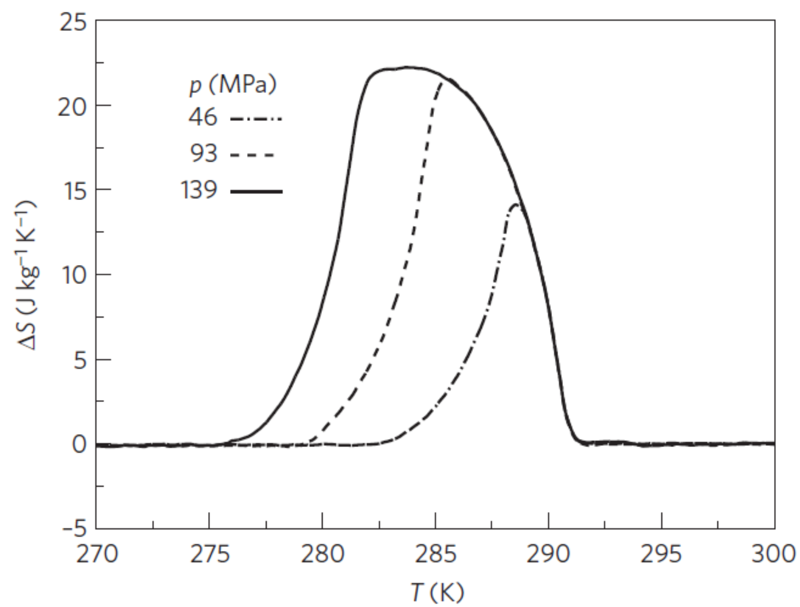


Mn-antiperovskites - Motivation

- Magnetocaloric effect in carbides (e.g., Mn_3GaC)
- Negative thermal expansion in nitrides (e.g., $Mn_3(Cu,Ge)N$, Mn_3NiN)
- Barocaloric effect in Mn_3GaN
- Piezomagnetic effect in Mn_3GaN (P. Lukashev et al., PRB 2008)



Wu et al., JAP 2013

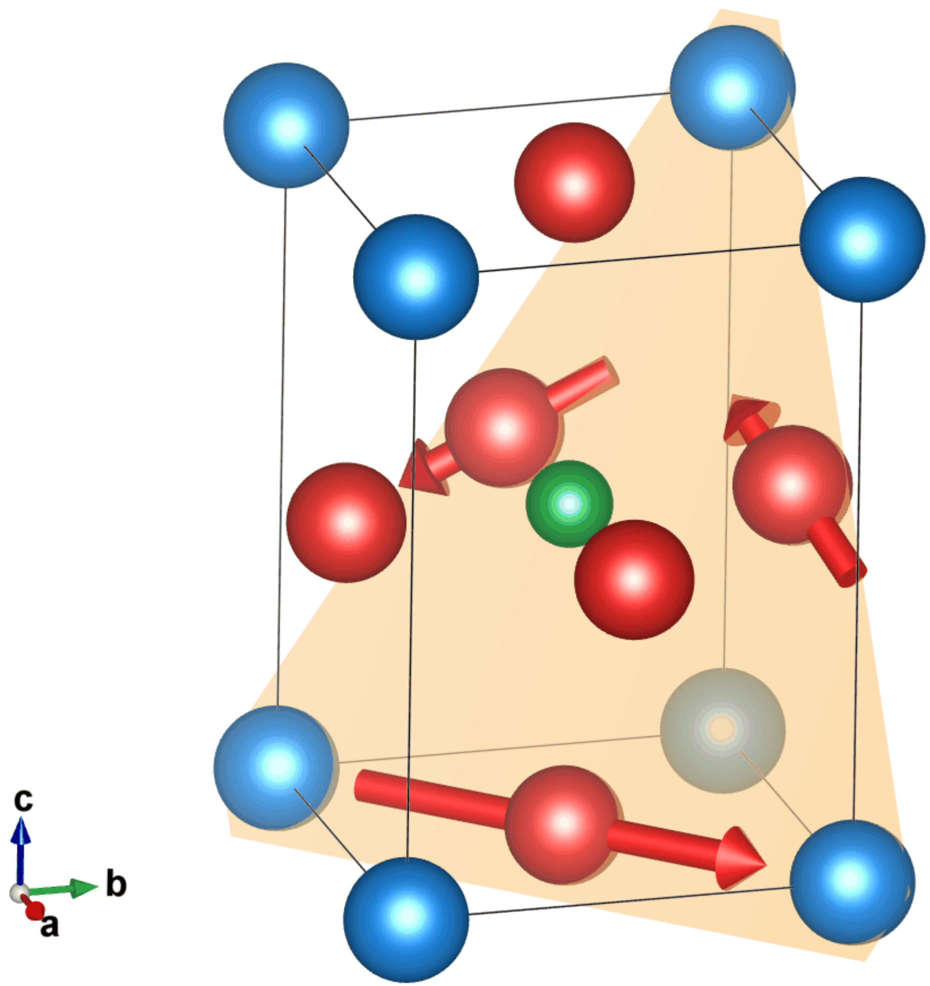


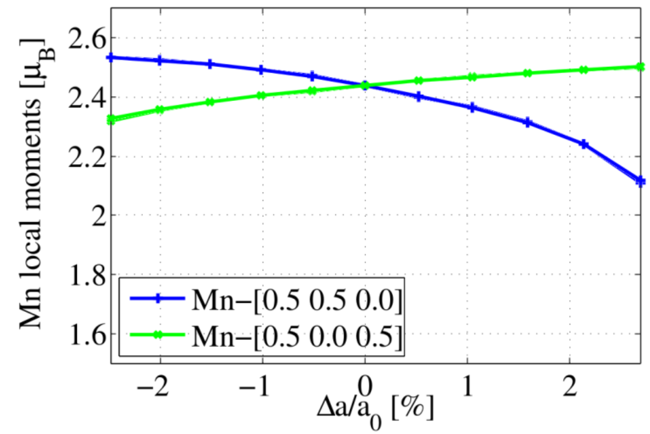
D. Matsunami, A. Fujita, K. Takenaka and M. Kano, Nat. Materials 2014

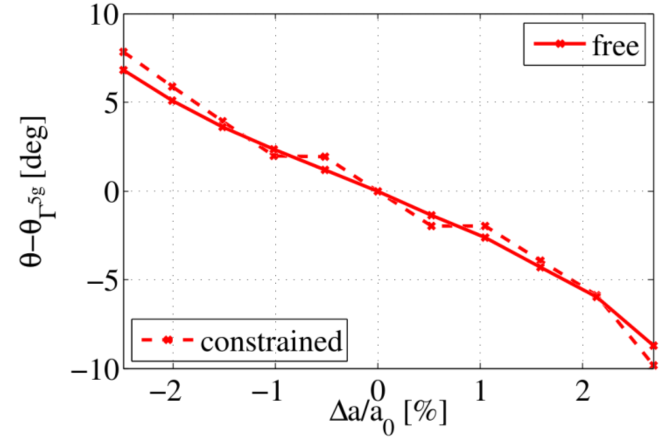
Outline

- Introduction
- Piezomagnetic effect (PME) – DFT simulations
- PME $\leftrightarrow$ magnetovolume & barocaloric effect
- Elastocaloric effect
- Outlook

Piezomagnetic effect - contributions



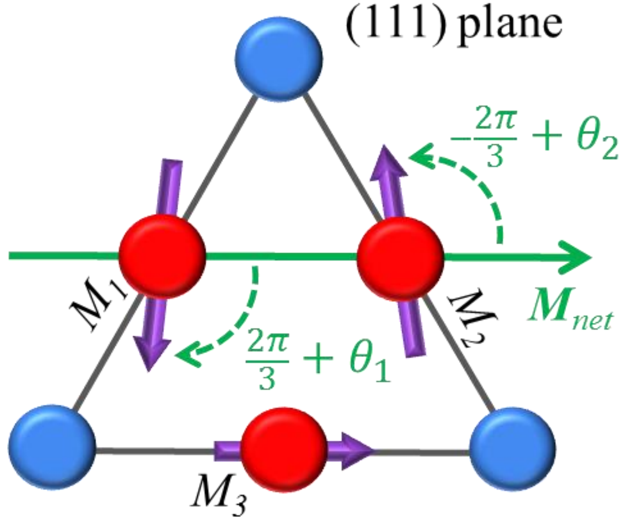




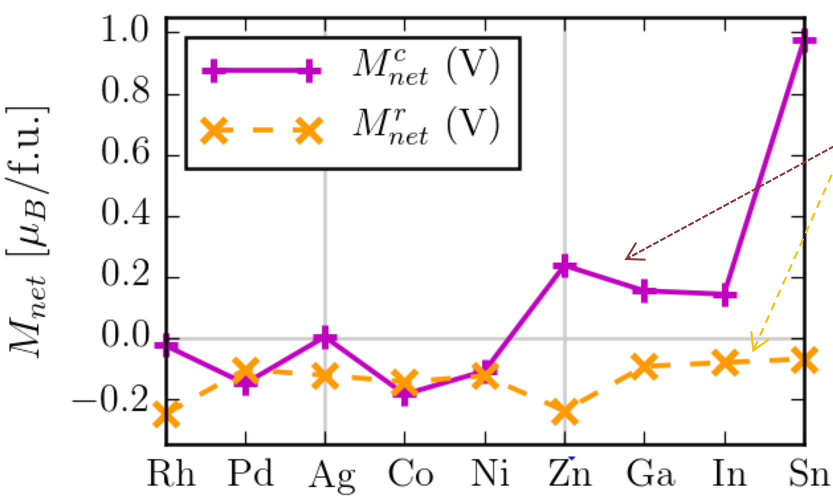
$$M_i = \underbrace{\lambda_{i,jk}\sigma_{jk}}_{piezo} + \underbrace{\mu_{i,jk}\sigma_{jk}^2}_{mag\text{-}elast} + \underbrace{\nu_{ijkl}\frac{\partial \sigma_{jk}}{\partial x_l}}_{flex};$$

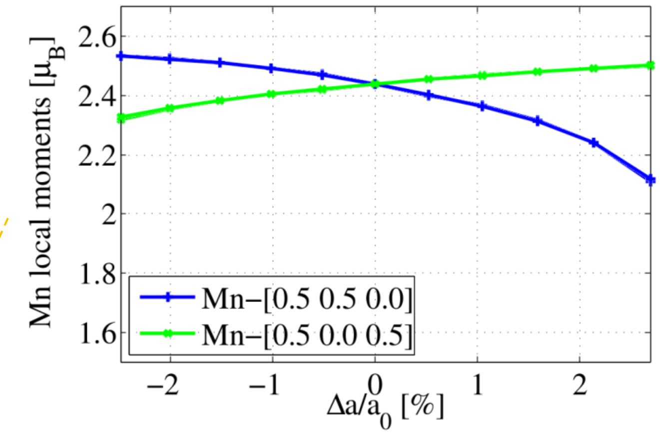
P. Lukashev et al., PRB 2010

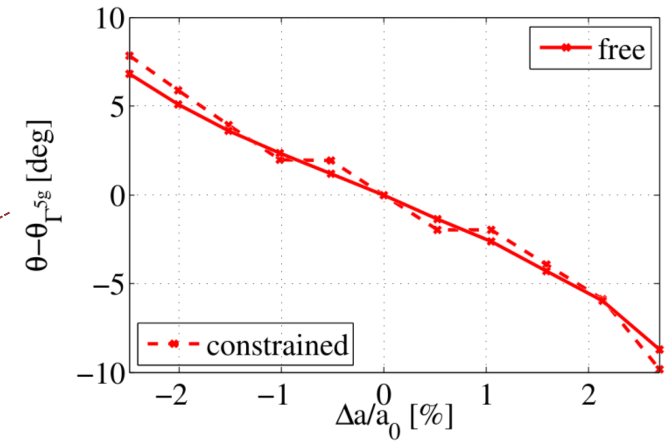
Piezomagnetic effect - contributions



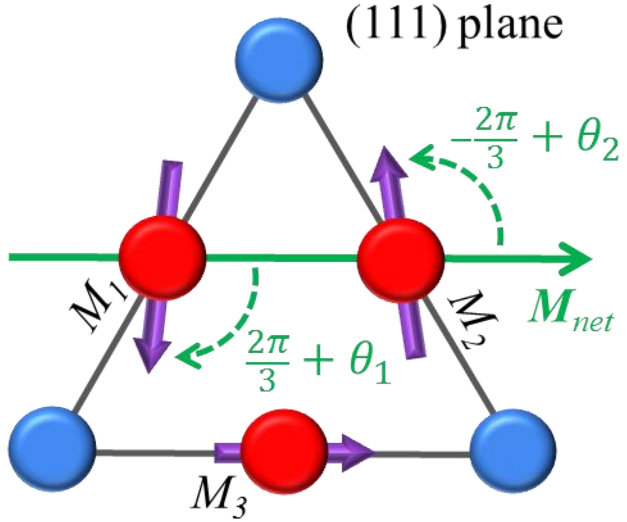
$$M^c_{net} \equiv 2M_0 \cos(2\pi/3 + \theta_1) + M_0,$$
$$M^r_{net} \equiv 2M_1 \cos(2\pi/3) + M_3 = M_3 - M_1$$





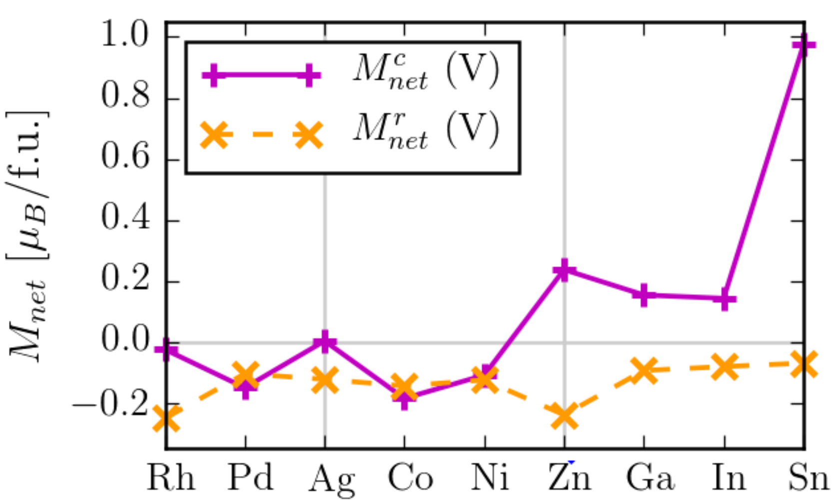


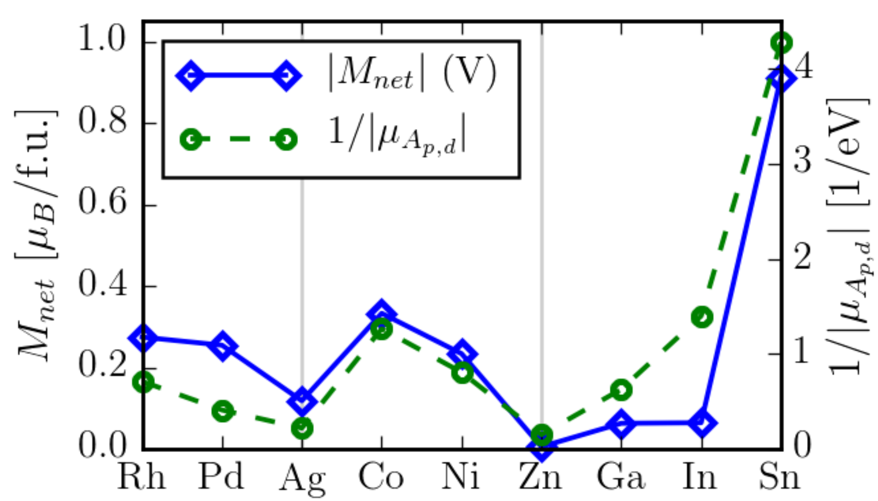
Piezomagnetic effect – net moment



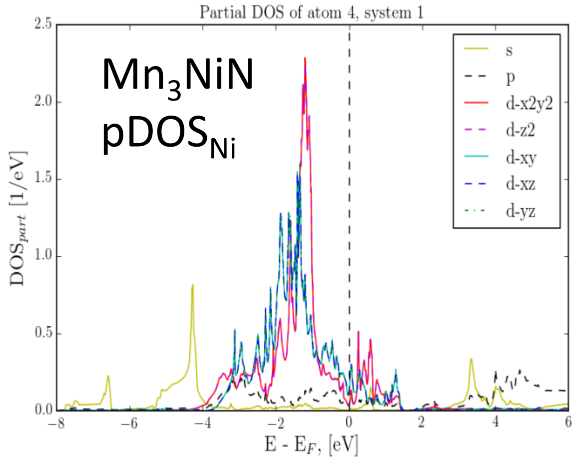
$$M^c_{net} \equiv 2M_0 \cos(2\pi/3 + \theta_1) + M_0,$$
$$M^r_{net} \equiv 2M_1 \cos(2\pi/3) + M_3 = M_3 - M_1$$

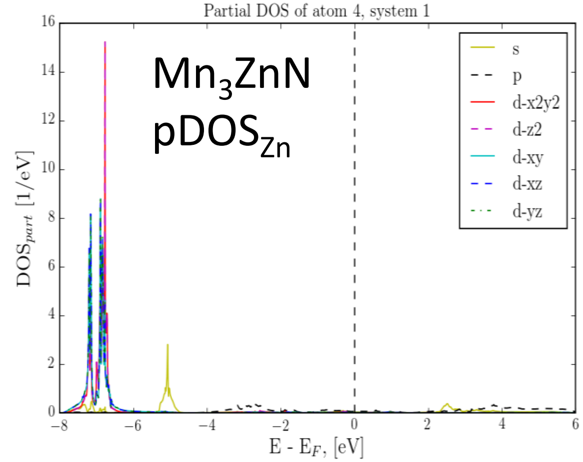
$$M_{net} = 2M_1 \cos(2\pi/3 + \theta_1) + M_3$$





Piezomagnetic effect – band structure





$$M^c_{net} \equiv 2M_0 \cos(2\pi/3 + \theta_1) + M_0,$$
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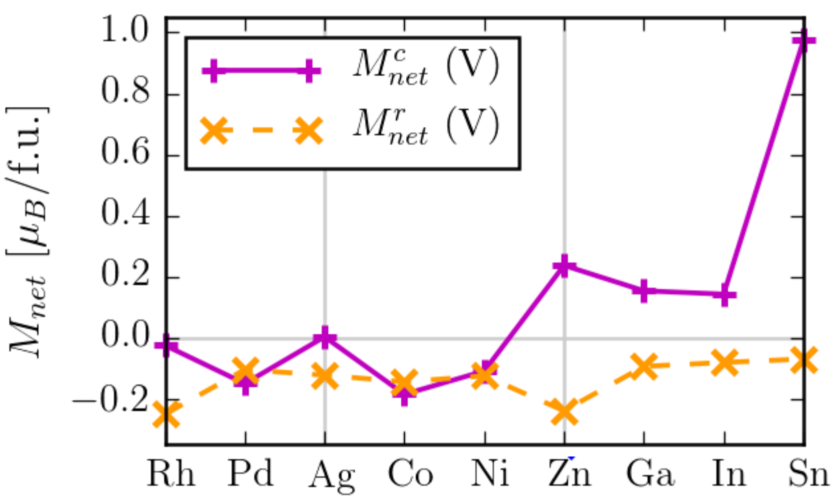
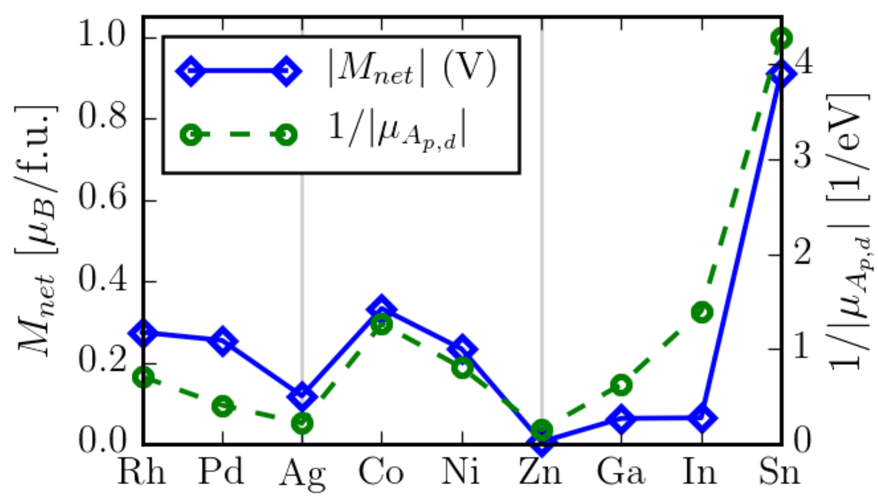
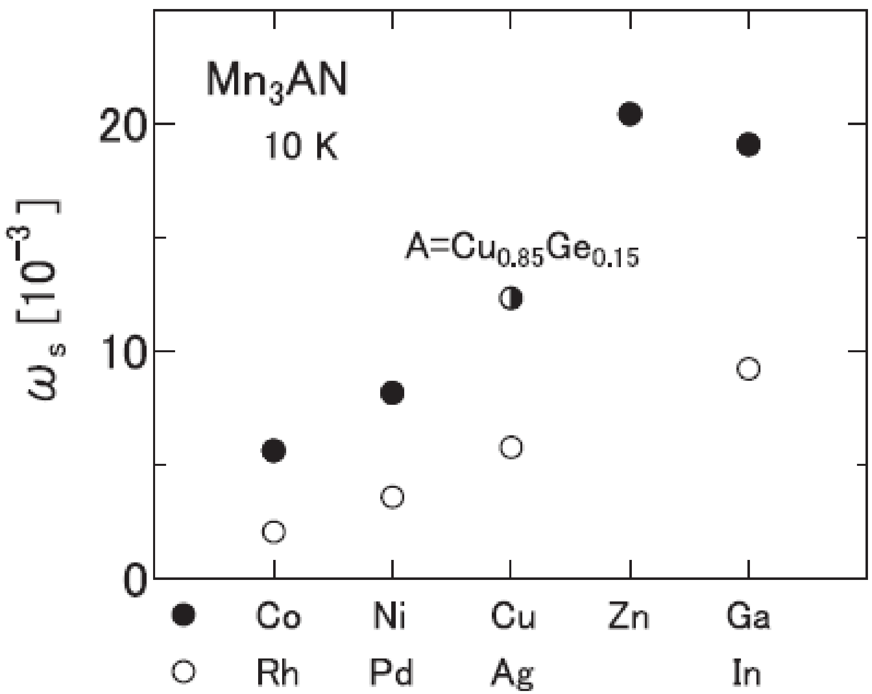
$$M_{net} = 2M_1 \cos(2\pi/3 + \theta_1) + M_3$$





Magnetovolume effect

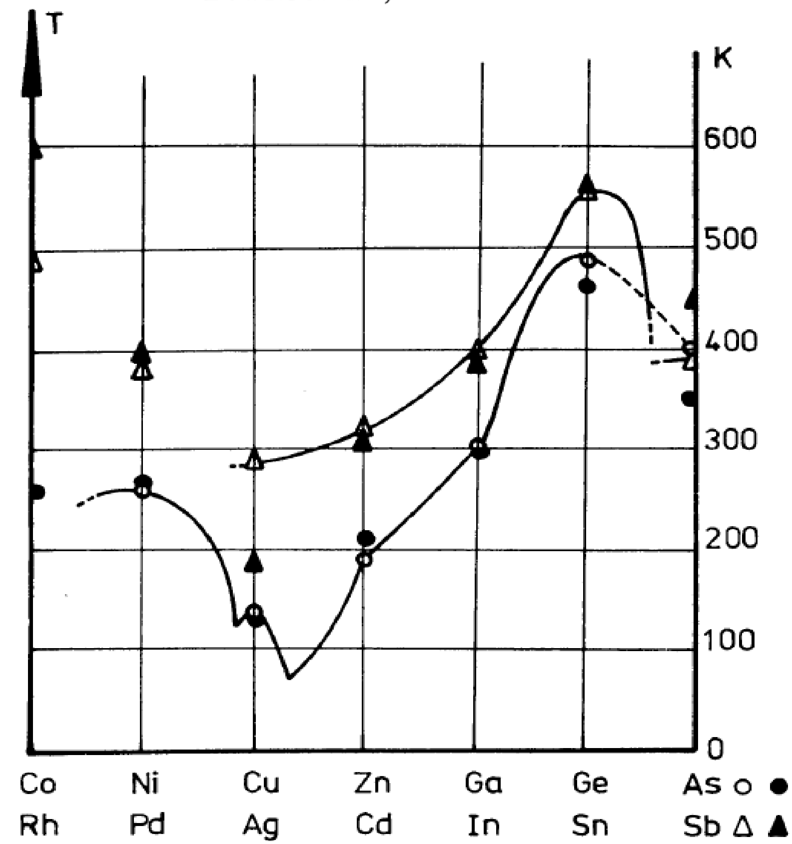
Koshi Takenaka et al.,
Sci. Technol. Adv. Mater. **15** (2014)



JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN, Vol. 44, No. 3, MARCH, 1978

Magnetic Studies of the Metallic Perovskite-Type Compounds of Manganese*

D. FRUCHART, E. F. BERTAUT

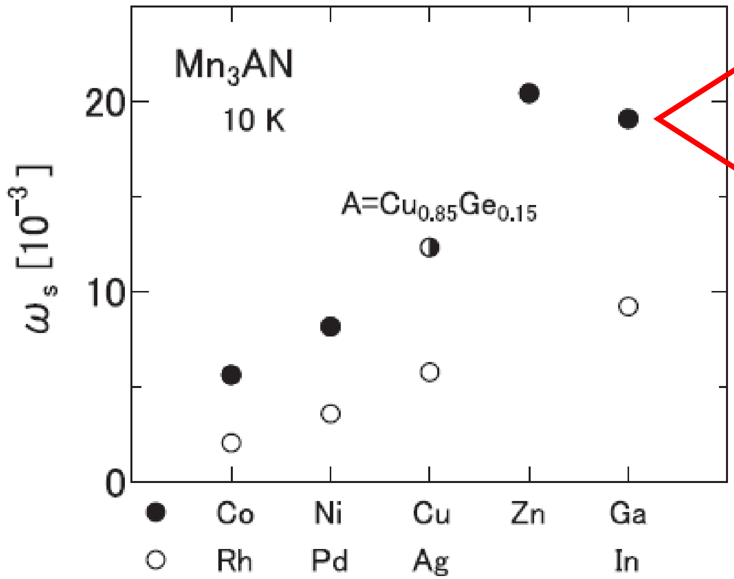


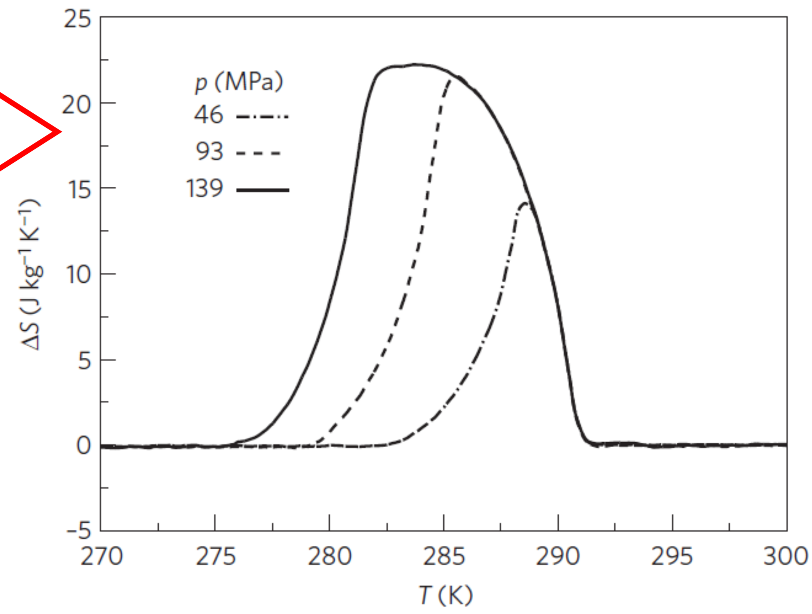
$$\zeta = K \cdot n_v (r_a + \Delta r_a)/r_a$$

Magnetovolume effect – barocaloric effect

Koshi Takenaka et al.,
Sci. Technol. Adv. Mater. (2014)

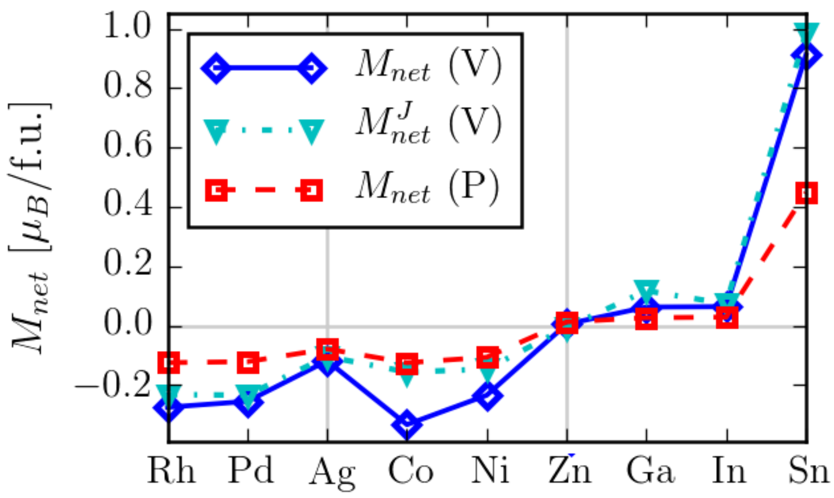
D. Matsunami, Koshi Takenaka et al.,
Nat. Materials (2014)





$$S(T_t, p) - S(T_t, 0) = V\omega_s \left(\frac{dT_t}{dp}\right)^{-1}$$

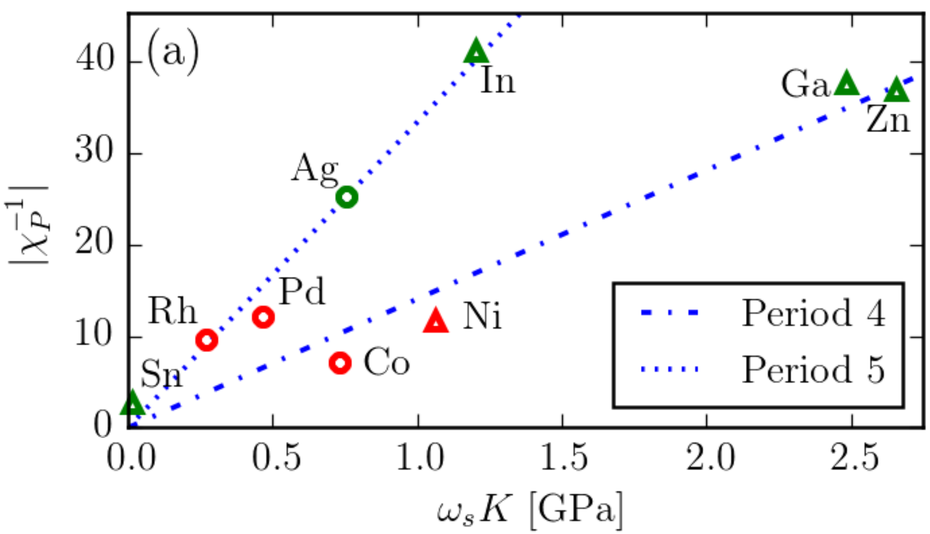
Piezomagnetic effect vs magnetovolume effect



$$\frac{M_{net}}{M_3} = 1 - \frac{J_{13}}{J_{12}}$$

$$\approx \frac{J_0 - \Delta J - (J_0 + \Delta J)}{J_0 - \Delta J} \approx -\frac{2\Delta J}{J_0}$$

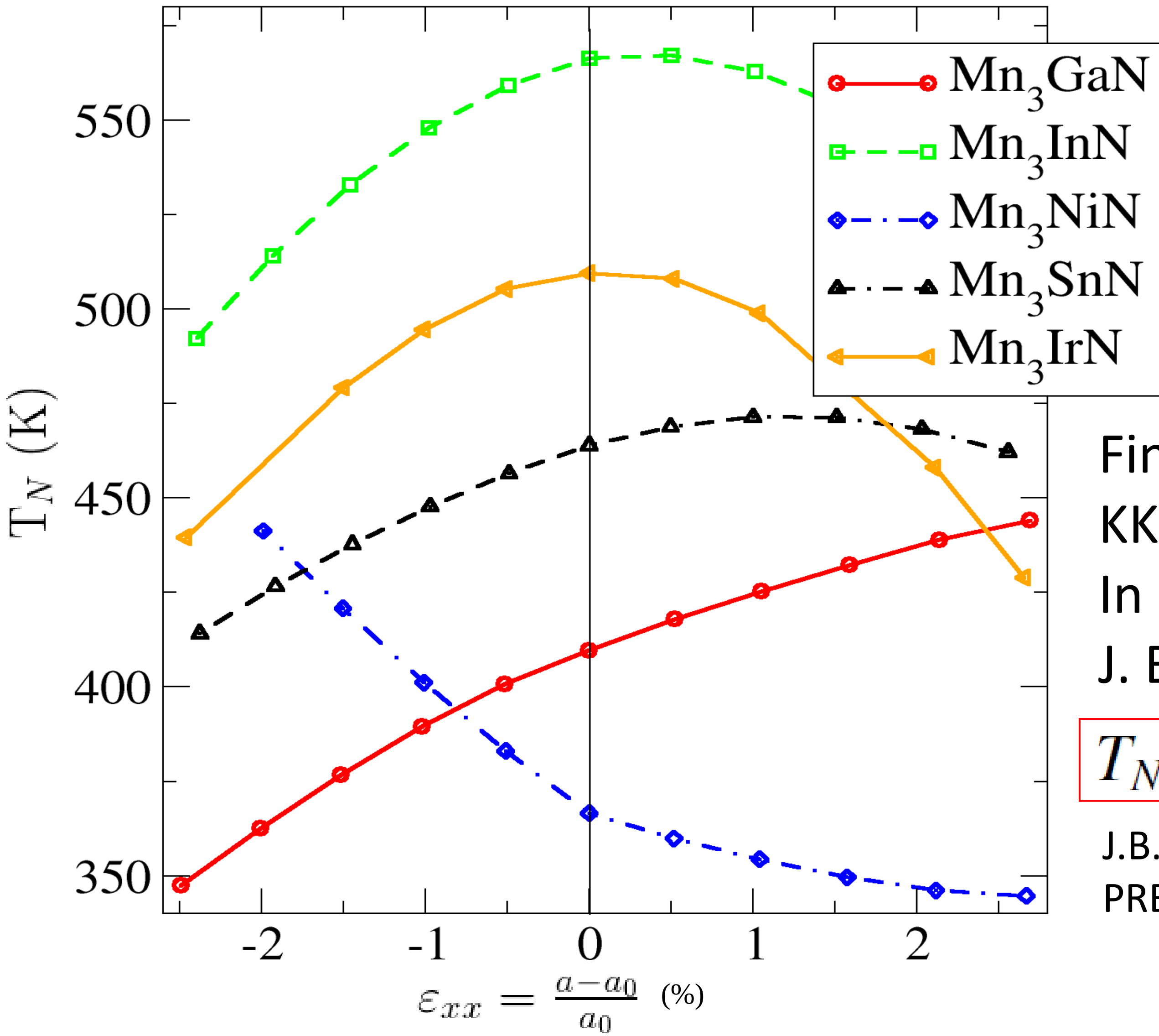
$$M^J_{net} \equiv -\frac{2M_3}{J_0}\Delta J = \frac{2M_3}{J_0}\frac{\partial J_{12}}{\partial \epsilon}\Delta\epsilon,$$



$$\frac{M^J_{net}}{M_3} = \frac{2}{J_0}\frac{\partial J_{12}}{\partial \epsilon}\Delta\epsilon \equiv \chi_P(\mu_{A_{p,d}})\Delta\epsilon$$

$$\omega_s K = -\frac{3M_0^2}{2V}\frac{\partial J_0}{\partial \omega}$$

Beyond the ground state - T_N(strain)



Finite temperature DFT:

KKR + DLM + $S^{(2)}$

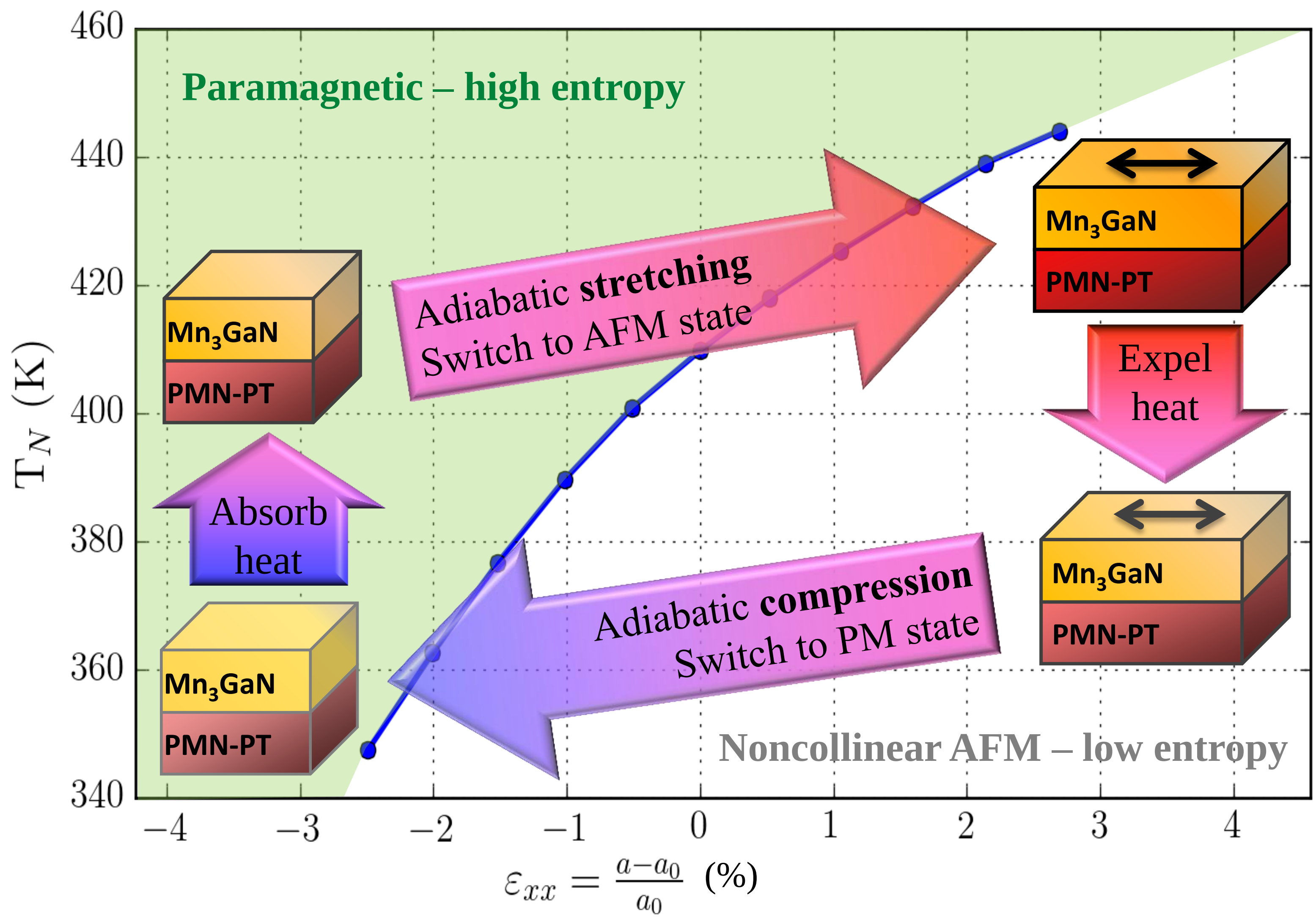
In collaboration with

J. B. Staunton

$$T_N = S^{(2)}(\vec{q}_{\max},0)/3k_B$$

J.B. Staunton et al.,
PRB **87**, 060404(R) (2013)

Elastocaloric cooling cycle – an alternative to magnetocaloric cooling (Rare earth free, driven by a piezo-stressor)



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Summary

- Identified Mn_3SnN as a material with large piezomagnetic effect at RT: dM= $0.5\mu_B$ per ε = 1%
- Related PME to electronic structure property
- Suggested a link between PME and MVE
- Explored train dependence of Néel temperature

- ToDo: strain induced entropy change (KKR-DLM)

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Thank you for your attention!