“Quiralidad en Magnetismo y Sistemas Cristalinos”

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Research Team

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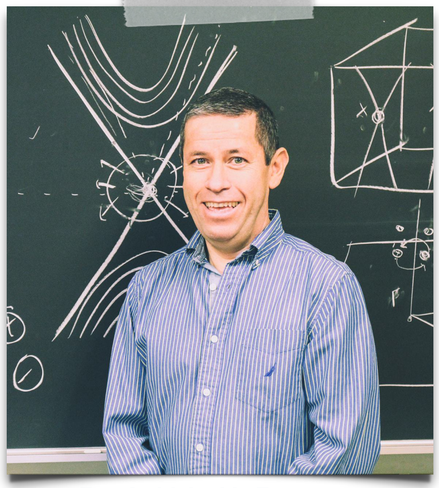
D. Torres-Amaris

Universidad Industrial de Santander



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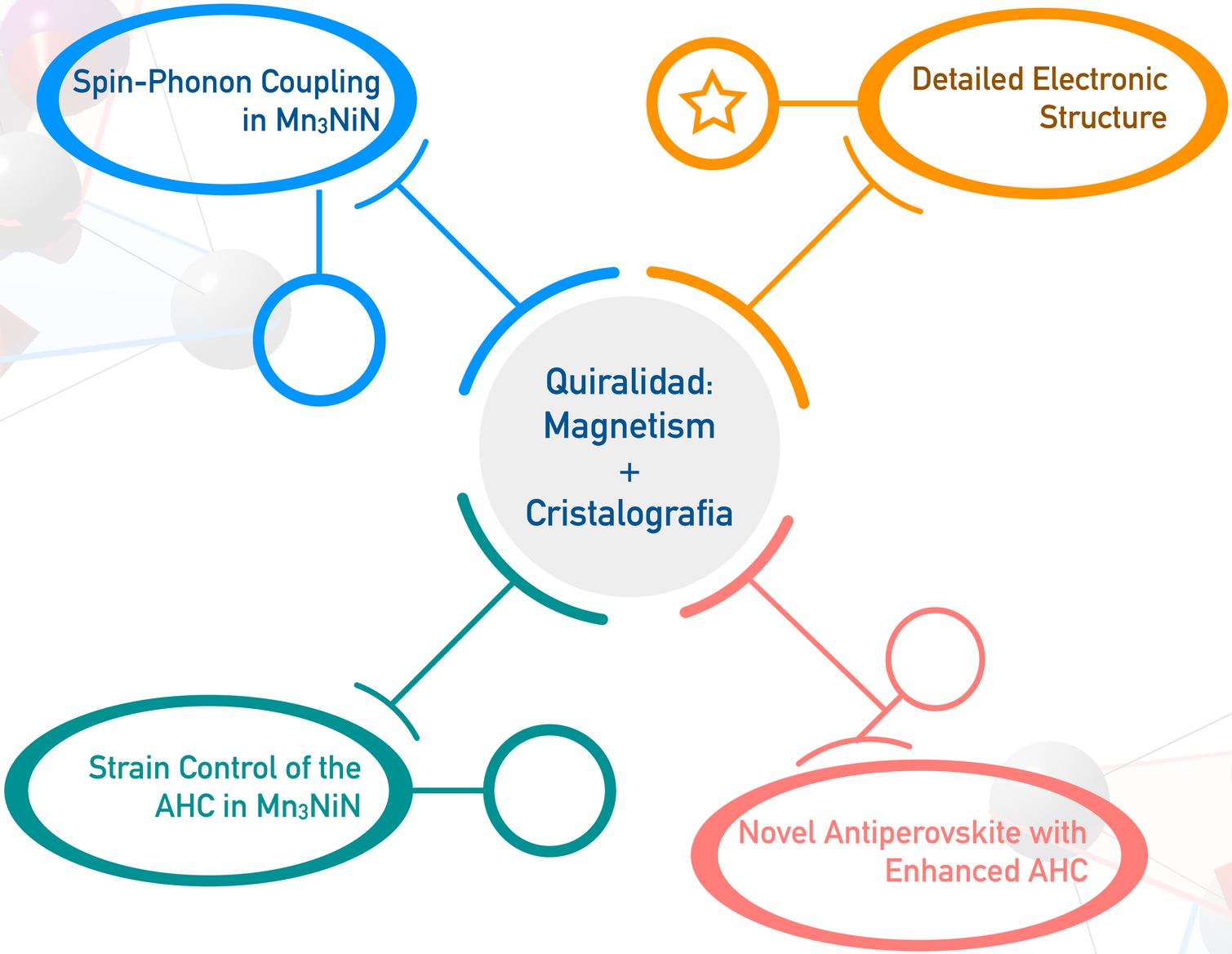
E. Triana-Ramirez

L. Gomez-Flores

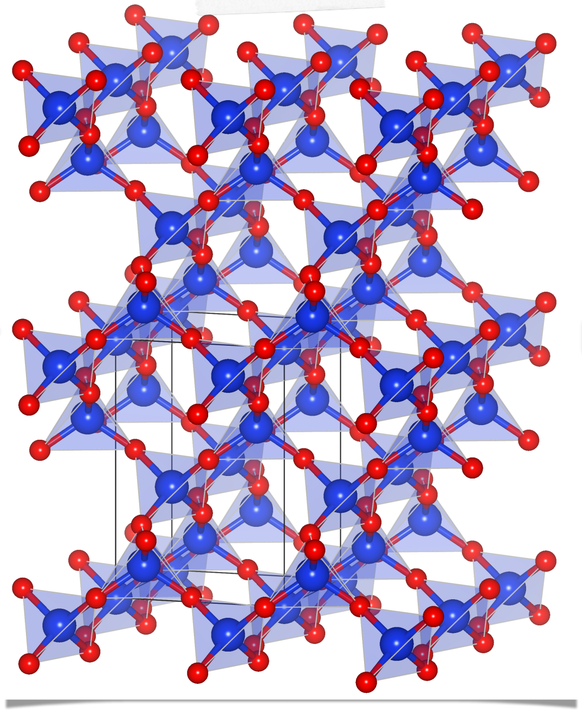
Cinvestav

Outline

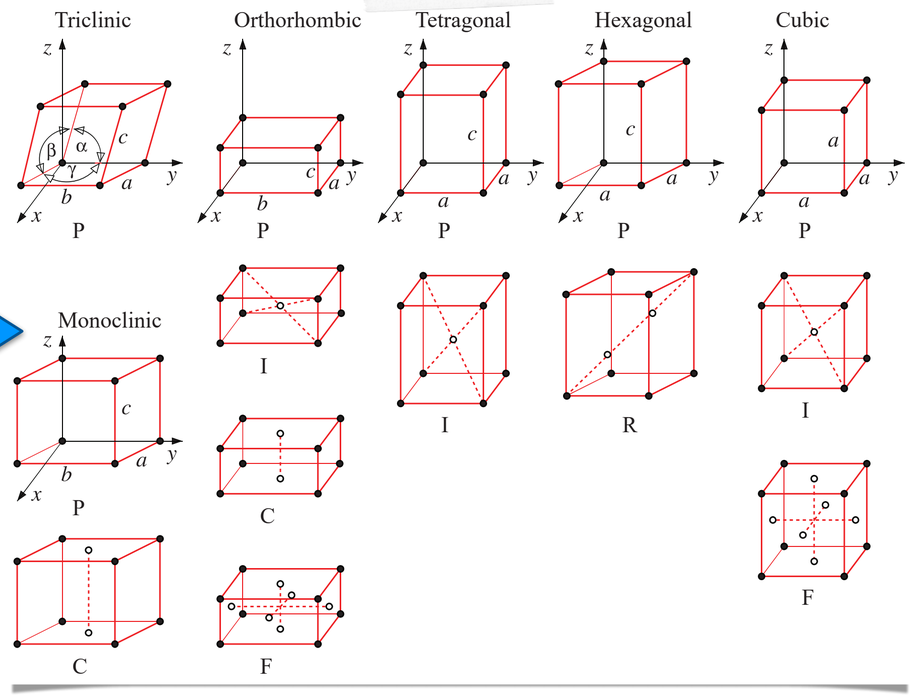

Spin-Phonon Coupling in Mn_3NiN
Detailed Electronic Structure
Quiralidad: Magnetism + Cristalografia
Strain Control of the AHC in Mn_3NiN
Novel Antiperovskite with Enhanced AHC

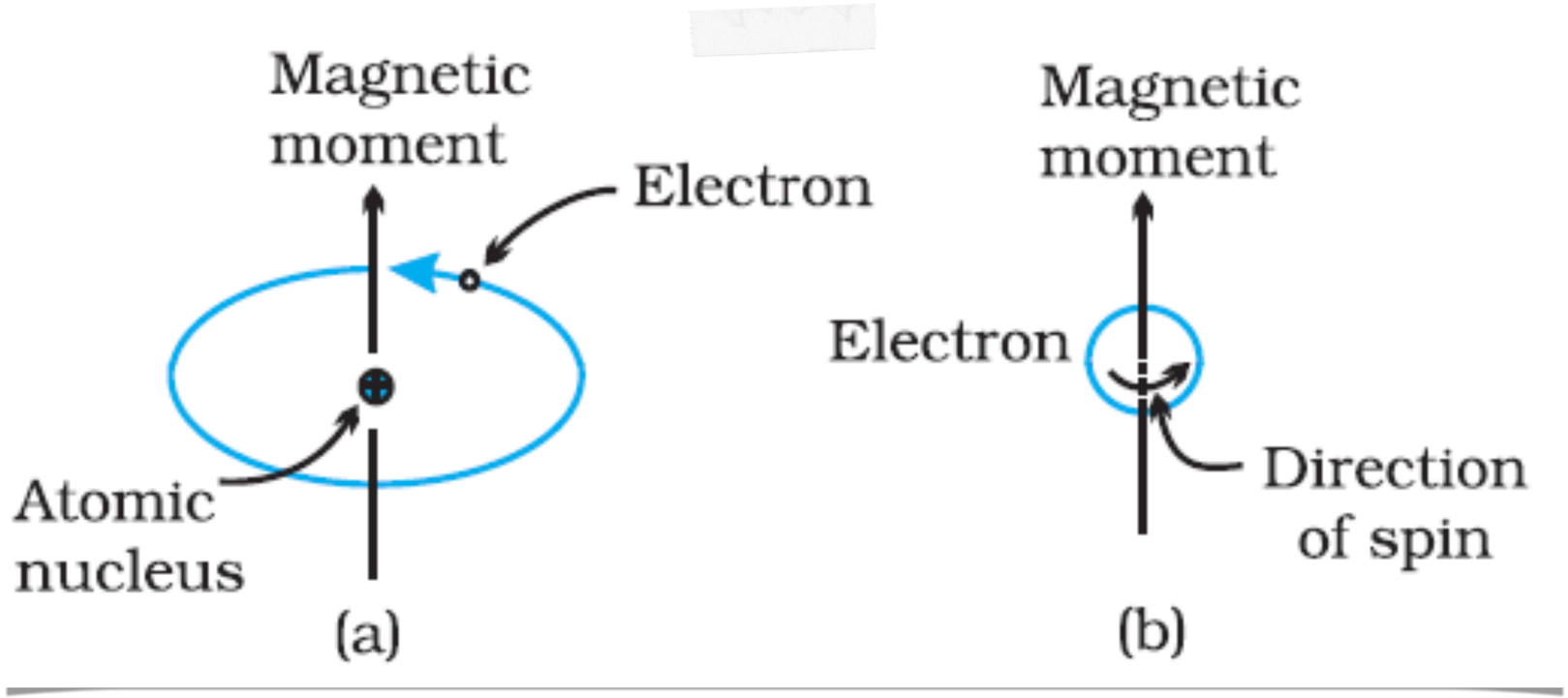
Amethist (SiO_2)

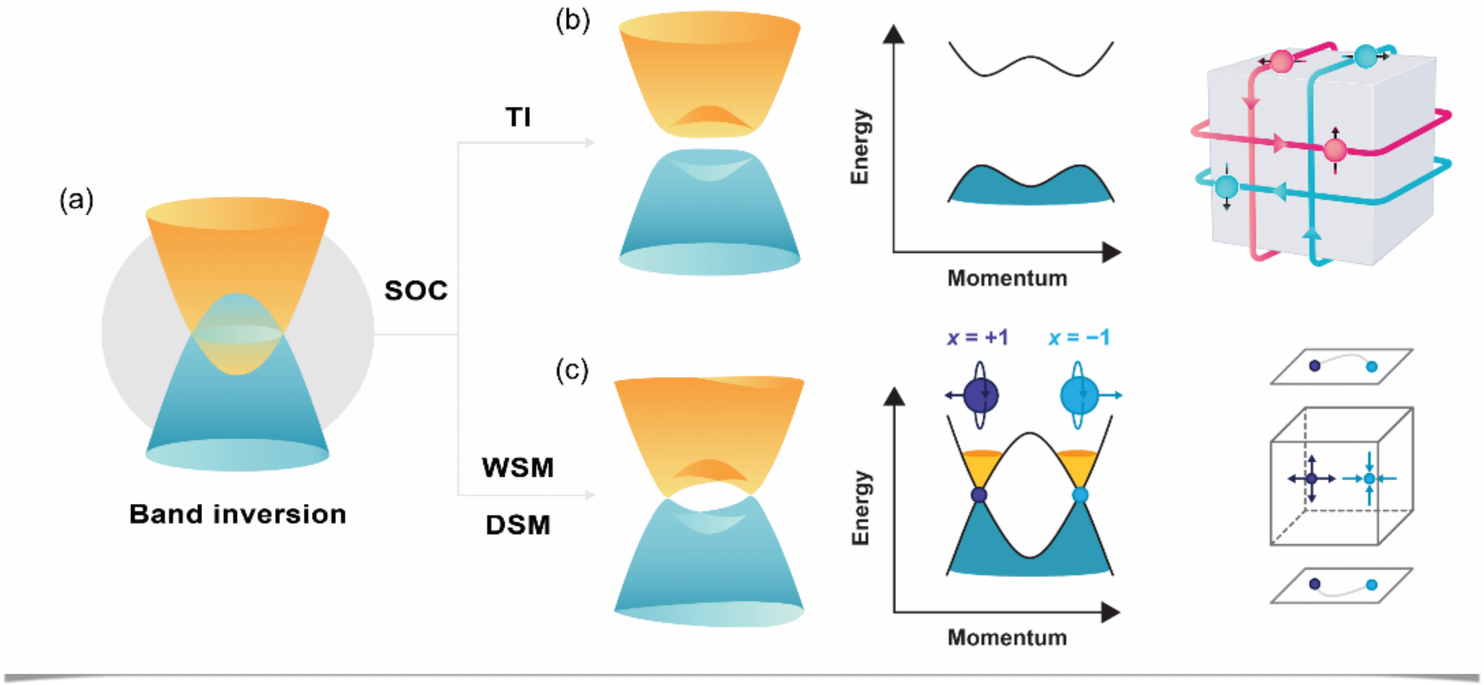
SiO_2 Lattice



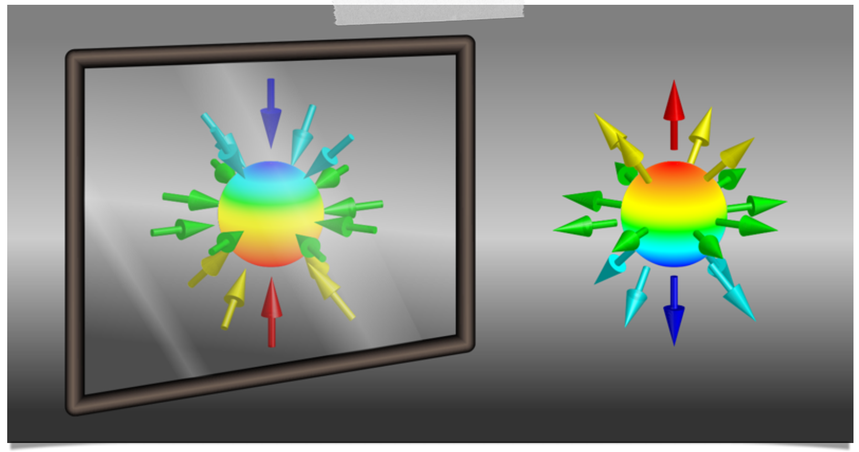
Bravais Lattices




Magnetic moment
Electron
Atomic nucleus
(a)
Magnetic moment
Electron
Direction of spin
(b)



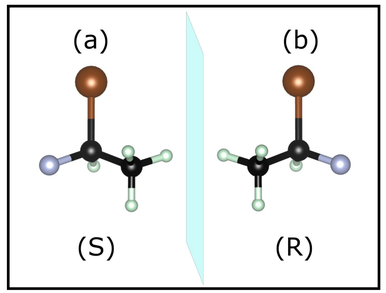
Claudia Feller and J. Gooth, ArXiv, arXiv:2205.05809 (2022).



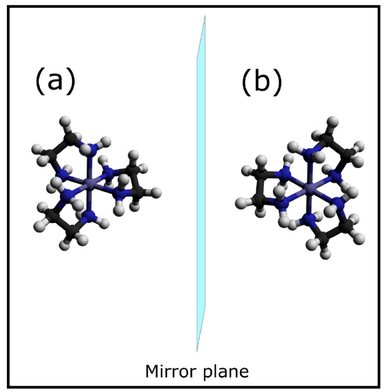
M. Sakano *et al.*, Phys. Rev. Lett. 124, 136404 (2020).

Chirality…

In chemistry



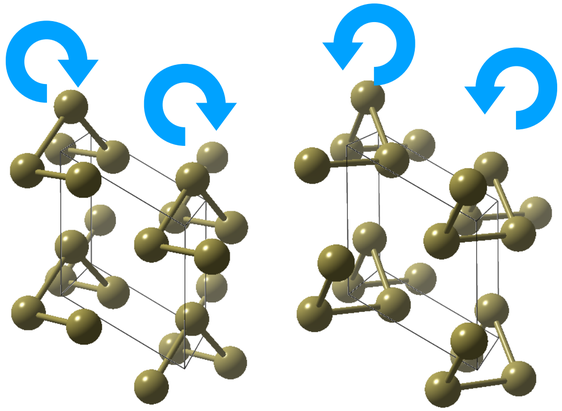
Enantiomers of 1Br-1Fluoroethane



tris(ethylenediamine)cobalt(III) Cloride
(a) Lambda and (b) Delta.

Enantiomers are molecules lacking of mirror and roto-inversion symmetries.

In crystals



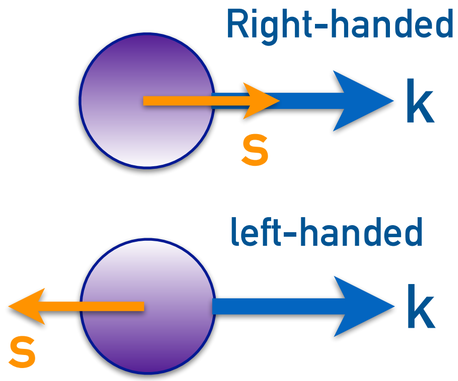
Te (SG. $P3_121$) Te (SG. $P3_221$)

Chang, Guoqing, et al. Nature materials 17,11 (2018).

M. Sakano et al. Phys. Rev. Lett., 124, 136404 (2020).

Chiral crystals lack of mirror and roto-reflexion symmetry.

In physics (particles and cosmology)



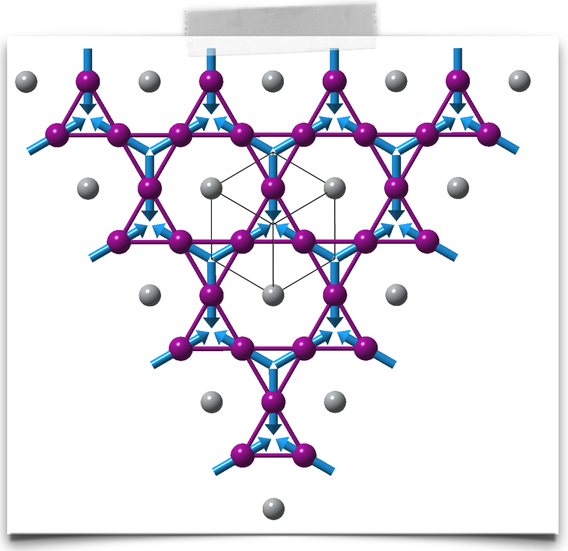
Determined by how the particle transform under parity transformation. (Accumulation of quantum phase)

Rober Cahn and Gerson Goldhaver, Cambridge University Press, (2009)

Kondepudi, D. K., & Durand, D. J. (2001).

In magnetism

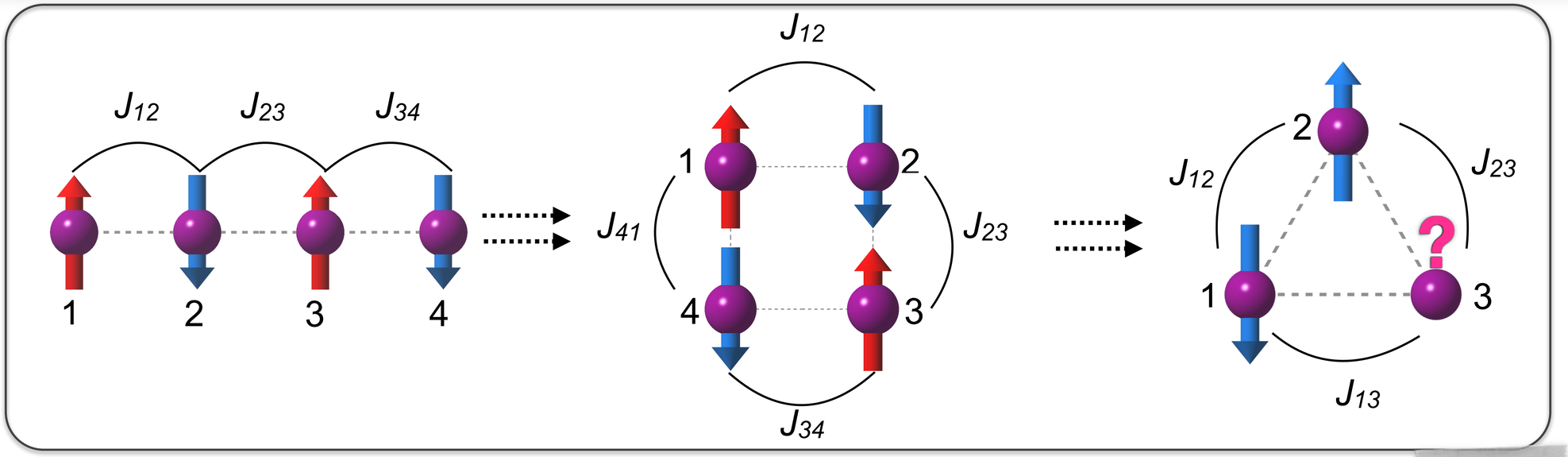
$$k = \frac{2}{3\sqrt{3}} \sum_{ij} \left[\vec{S}_i \times \vec{S}_j \right]_z$$



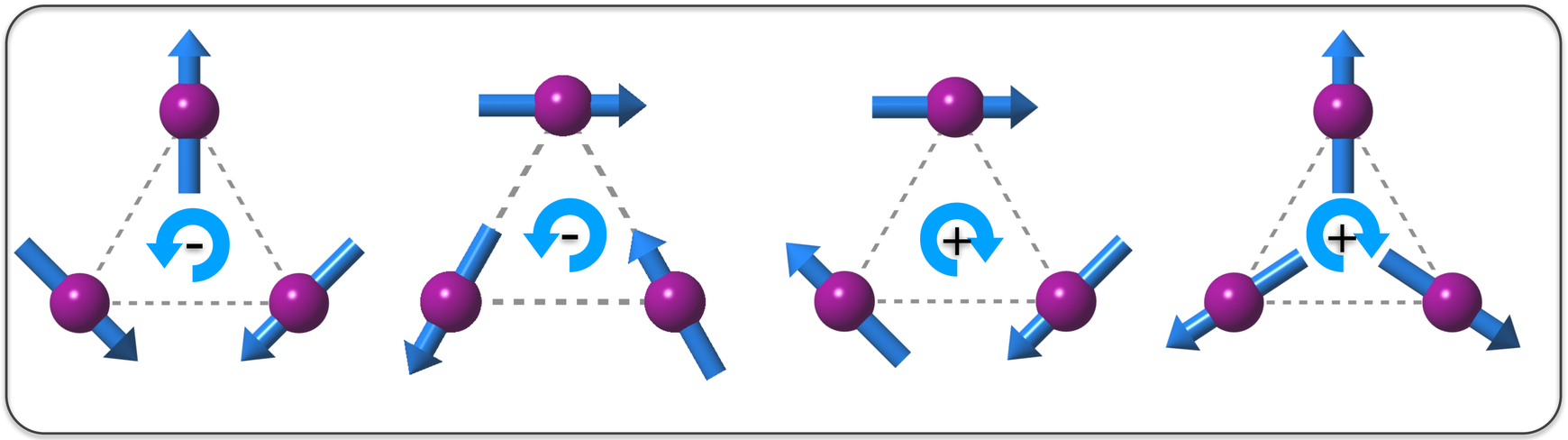
A. P. Ramirez, Annu. Rev. Mater. Sci. 24, 453-480, (1994).

Results from the magnetic ordering that could break the rotational symmetry.

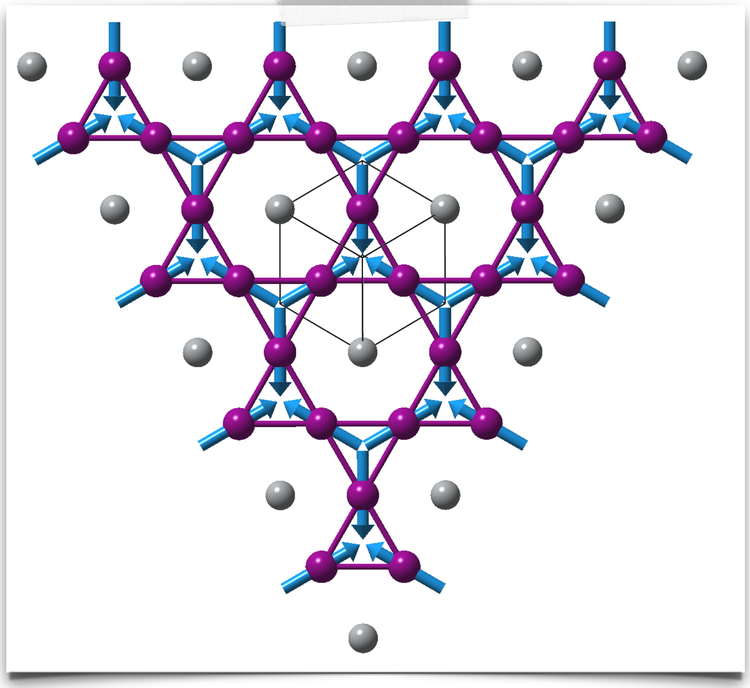
Magnetic Frustration and Magnetic Chirality



A. P. Ramirez, Annu. Rev. Mater. Sci. 24, 453-480, (1994).

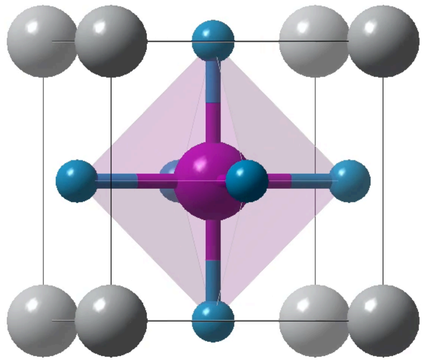


D. Fruchart and E. F. Bertaut, Journal of the Physical Society of Japan, 44, 781 (1978).

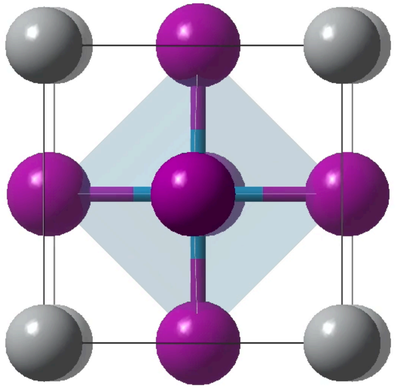


Kagome lattice

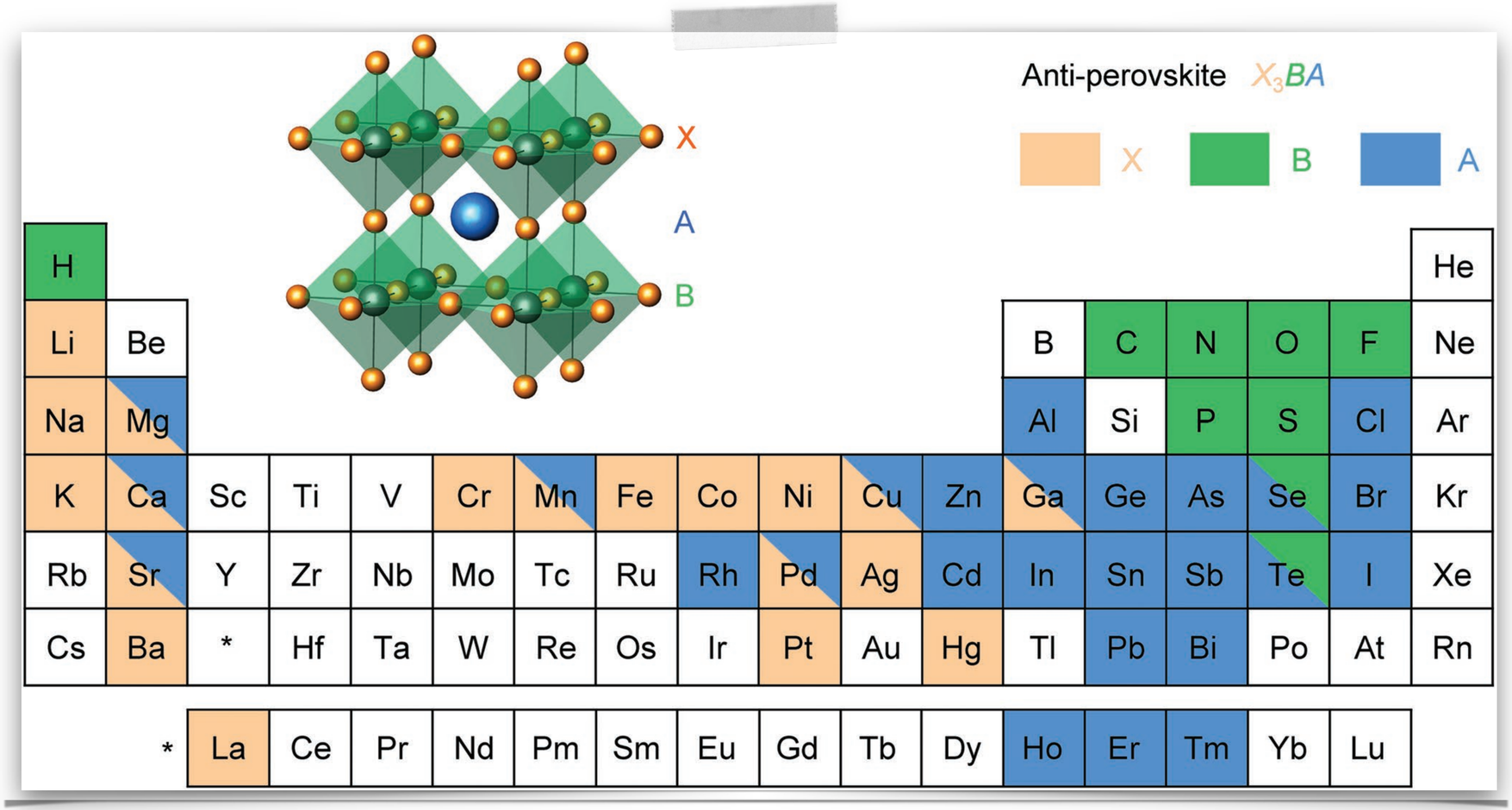
Antiperovskites…!



Perovskite ABX_3



Antiperovskite A_3BX



Y. Wang, et al. Adv. Mater. 1905007, 1 (2019).

REVIEW

ADVANCED MATERIALS
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Antiperovskites with Exceptional Functionalities

Yonggang Wang, Hao Zhang, Jinlong Zhu, Xujie Lü, Shuai Li, Ruqiang Zou, and Yusheng Zhao**

PHYSICAL REVIEW B **100**, 094426 (2019)

Topology analysis for anomalous Hall effect in the noncollinear antiferromagnetic states of Mn_3AN (A = Ni, Cu, Zn, Ga, Ge, Pd, In, Sn, Ir, Pt)

Vu Thi Ngoc Huyen,[1,2,3] Michi-To Suzuki,[4,*] Kunihiko Yamauchi,[1] and Tamio Oguchi[1,2]
[1]*Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan*
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[3]*Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan*
[4]*Center for Computational Materials Science, Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan*

Superconductivity in the non-oxide perovskite $MgCNi_3$

T. He*, Q. Huang†, A. P. Ramirez‡, Y. Wang§, K. A. Regan*, N. Rogado*, M. A. Hayward*, M. K. Haas*, J. S. Slusky*, K. Inumara*, H. W. Zandbergen*, N. P. Ong§ & R. J. Cava*

** Department of Chemistry and Princeton Materials Institute; § Department of Physics, Princeton University, Princeton, New Jersey, USA*
† Department of Materials and Nuclear Engineering, University of Maryland, College Park, Maryland; and NIST Center for Neutron Research, Gaithersburg, Maryland, USA
‡ Condensed Matter and Thermal Physics Group, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

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Superionic Conductivity in Lithium-Rich Anti-Perovskites

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Sci. Technol. Adv. Mater. **15** (2014) 015009 (11pp) — doi:10.1088/1468-6996/15/1/015009

Magnetovolume effects in manganese nitrides with antiperovskite structure

Koshi Takenaka[1,2], Masayoshi Ichigo[1], Taisuke Hamada[1], Atsushi Ozawa[1], Takashi Shibayama[1], Tetsuya Inagaki[1] and Kazuko Asano[1]

[1] Department of Crystalline Materials Science, Nagoya University, Nagoya 464-8603, Japan
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ARTICLE

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DOI: 10.1038/ncomms13617 OPEN

Superconductivity in the antiperovskite Dirac-metal oxide $Sr_{3-x}SnO$

Mohamed Oudah[1], Atsutoshi Ikeda[1], Jan Niklas Hausmann[1,2], Shingo Yonezawa[1], Toshiyuki Fukumoto[3], Shingo Kobayashi[3,4], Masatoshi Sato[5] & Yoshiteru Maeno[1]

SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

Epitaxial antiperovskite/perovskite heterostructures for materials design

Camilo X. Quintela[1], Kyung Song[2], Ding-Fu Shao[3], Lin Xie[4], Tianxiang Nan[1], Tula R. Paudel[3], Neil Campbell[5], Xiaoqing Pan[6], Thomas Tybell[7], Mark S. Rzchowski[5], Evgeny Y. Tsymbal[3], Si-Young Choi[8]*, Chang-Beom Eom[1]*

How we perform the study… The magic of DFT…!

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle\,,$$

$$\hat{H}(\mathbf{R},\mathbf{r}) = \hat{T}_N(\mathbf{R}) + \hat{T}_e(\mathbf{r}) + \hat{V}_{NN}(\mathbf{R}) + \hat{V}_{ee}(\mathbf{r}) + \hat{V}_{eN}(\mathbf{r},\mathbf{R}),$$

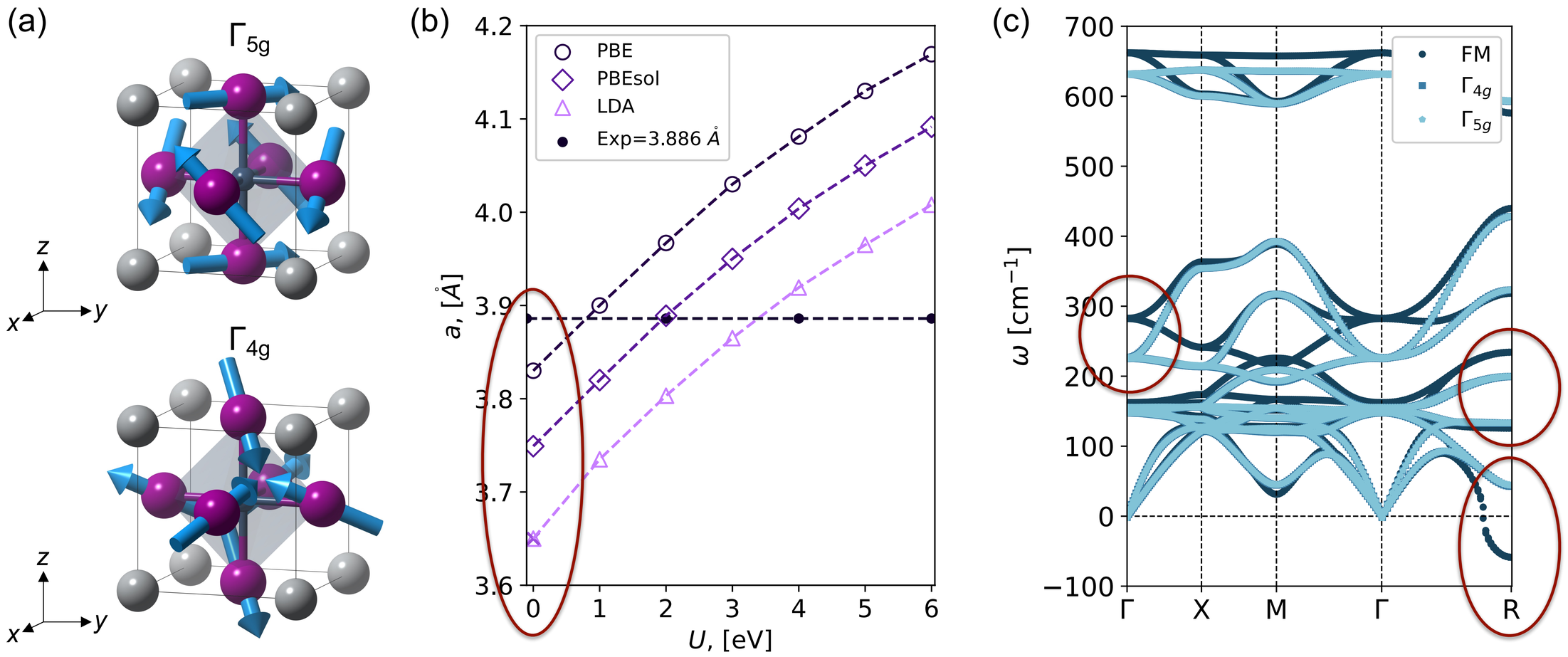
$$\hat{H}_e = \hat{T}_e + \hat{V}_{ee} + \hat{V}_{ext} = \hat{T}_e + \hat{V}_{ee} + \sum_i v(\mathbf{r}_i).$$

$$\begin{aligned} E[n(\mathbf{r})] &= \langle\Psi_e|\,\hat{T}_e + \hat{V}_{ee}\,|\Psi_e\rangle + \langle\Psi_e|\,\hat{V}_{ext}\,|\Psi_e\rangle \\ &= F[n(\mathbf{r})] + \int v(\mathbf{r})n(\mathbf{r})\,d\mathbf{r}, \end{aligned}$$

Theorem 1: *The ground-state energy from Schrödinger's equation is a unique functional of the electron density* [31].

Theorem 2: *The electron density that minimizes the energy of the overall functional is the true electron density corresponding to the full solution of the Schrödinger's equation* [31].

Electron- and spin-phonon coupling

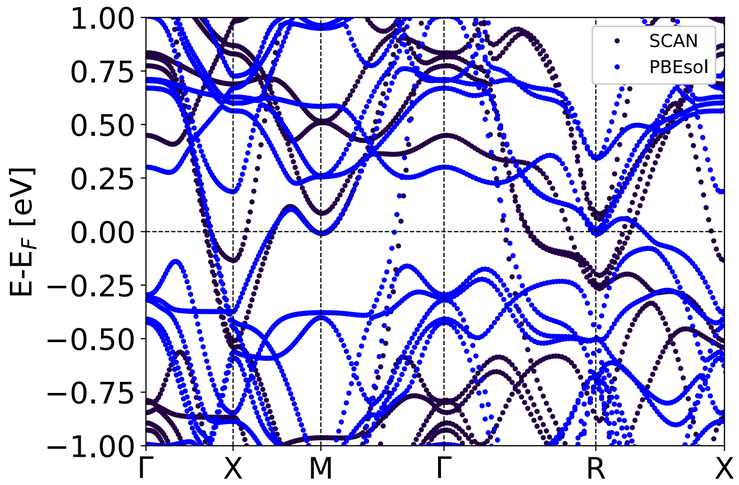


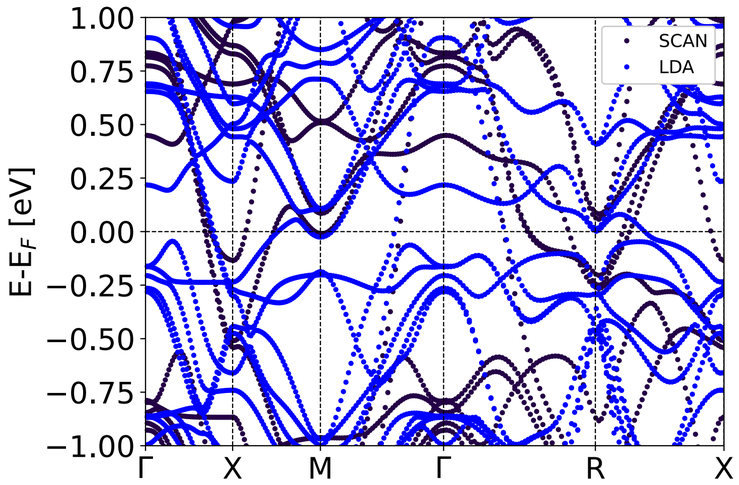
D. Fruchart and E. F. Bertaut, Journal of the Physical Society of Japan, 44, 781 (1978).

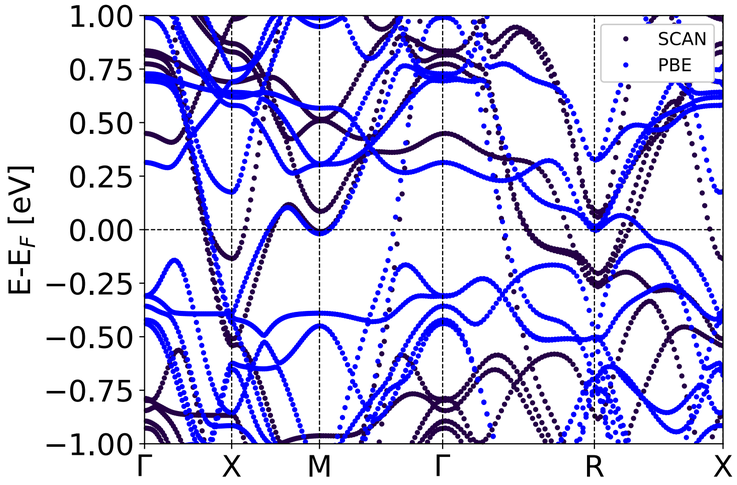
L. Flores-Goméz, *et. al.*, J. Mag. Mag. Mat. 562, 169813, (2022).

Electron- and spin-phonon coupling

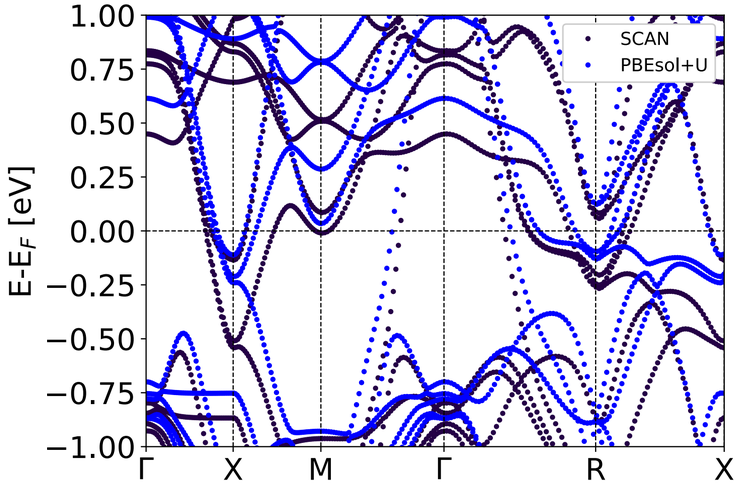
First…! Theoretical approach? Most used in the literature

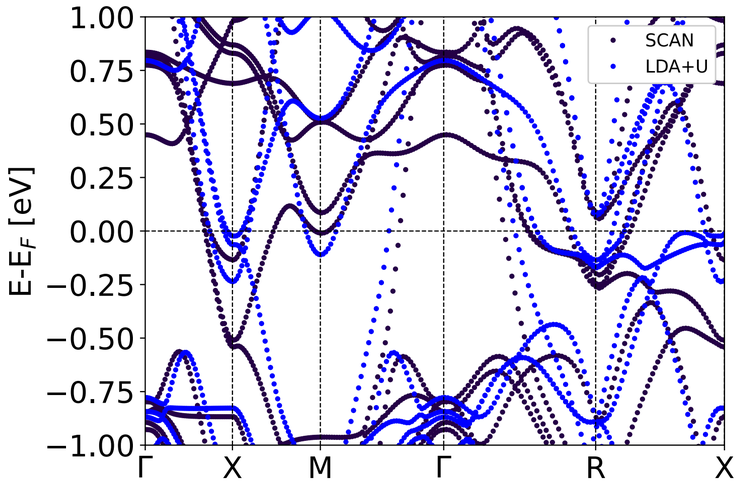


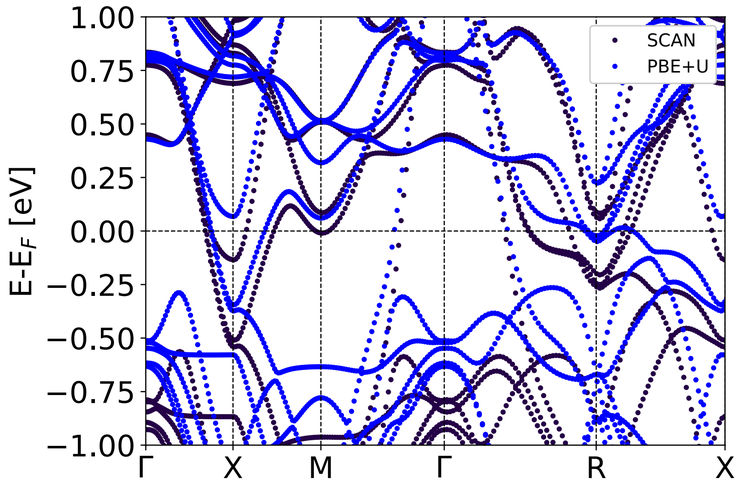




Theoretical corrections…?

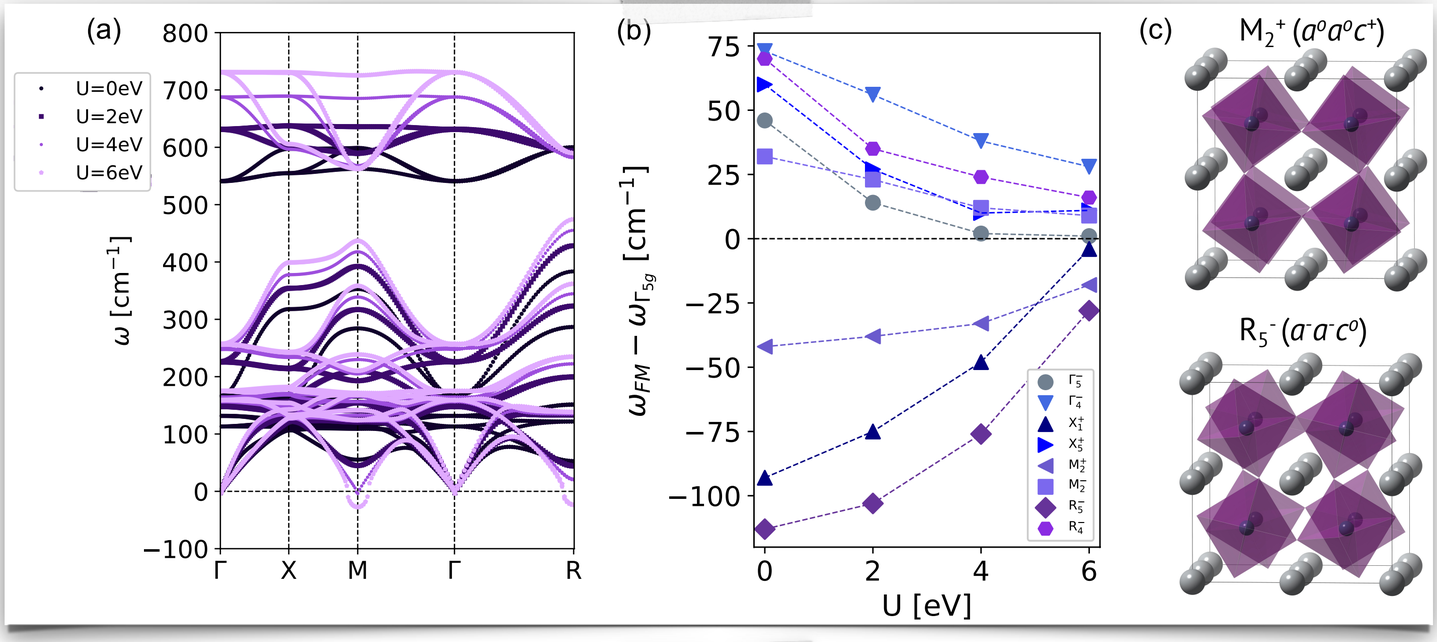


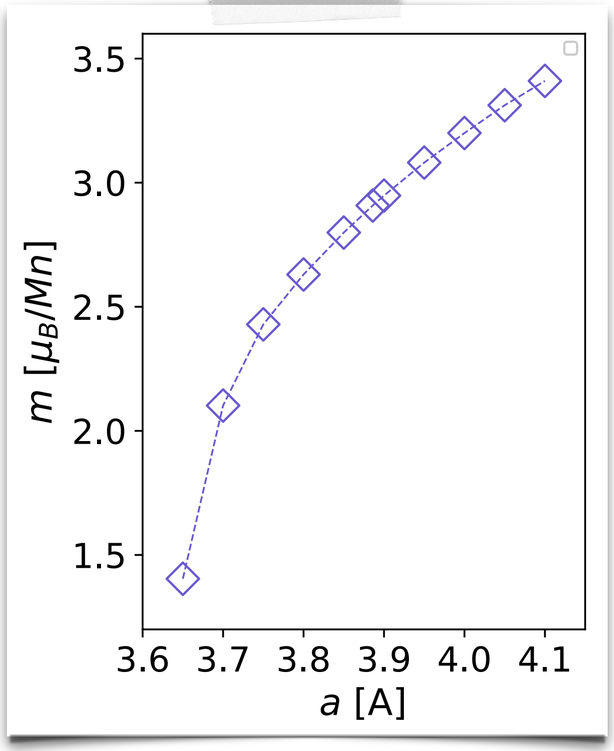


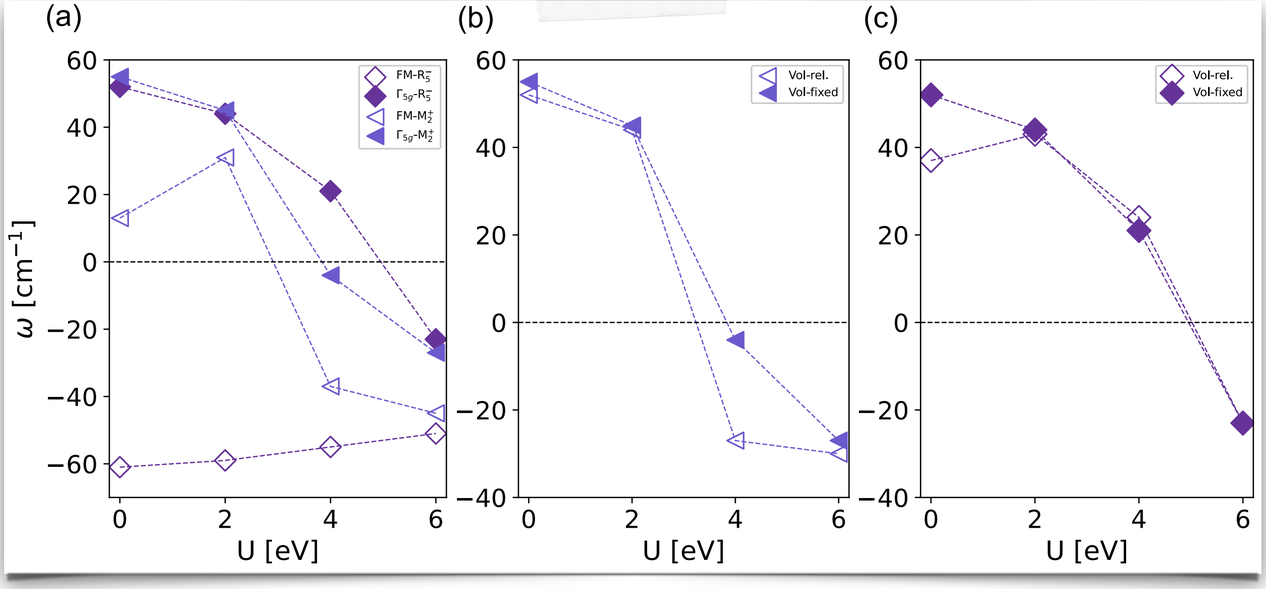


L. Flores-Goméz, *et. al.*, J. Mag. Mag. Mat. 562, 169813, (2022).

Electron- and spin-phonon coupling





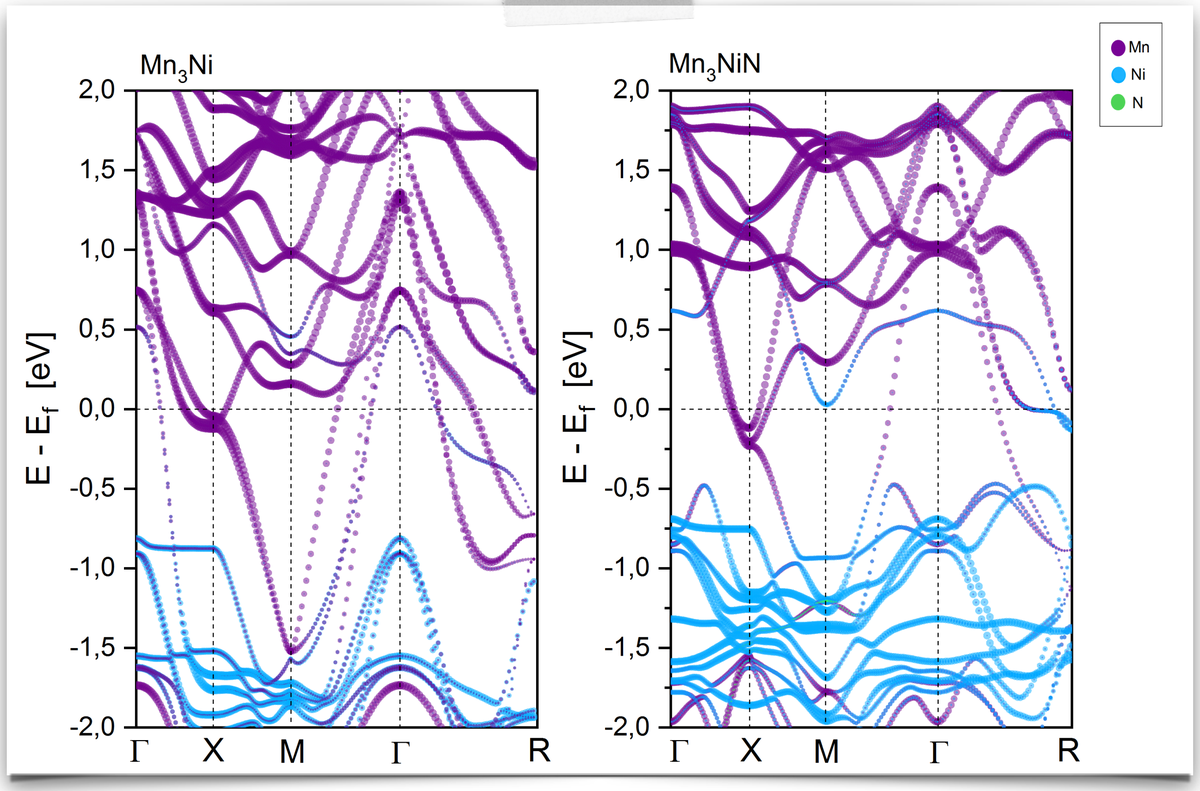


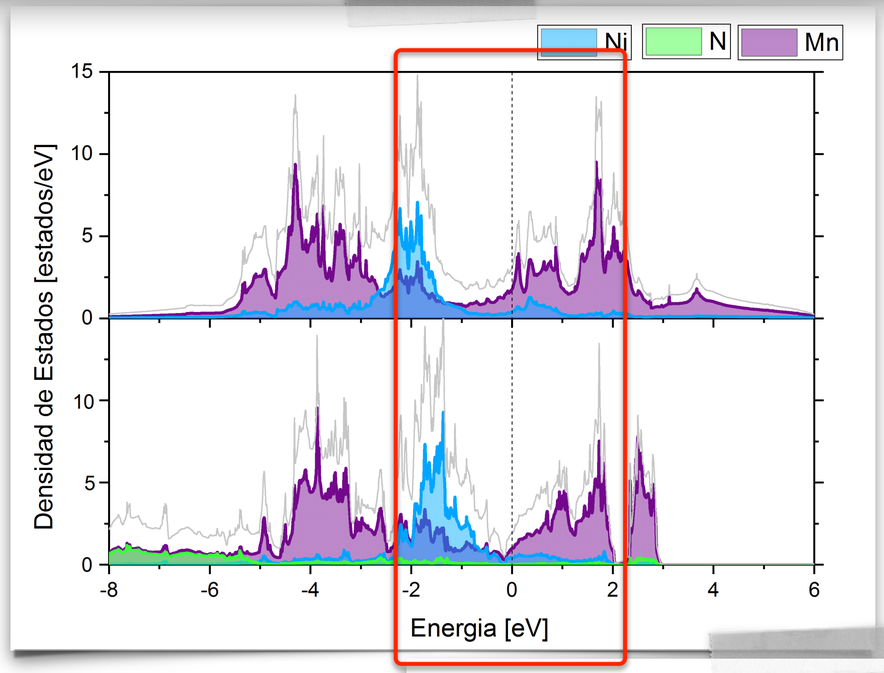
Phonons modulated by the exchange coupling and the volume effects…!

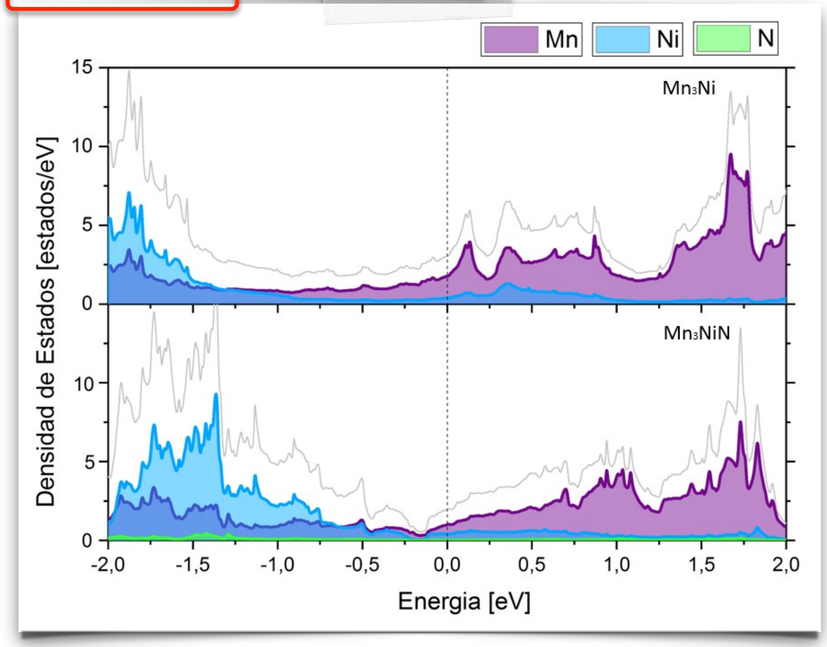
L. Flores-Goméz, *et. al.*, J. Mag. Mag. Mat. 562, 169813, (2022).

What about their electronic structure…?

Detailed Electronic Structure: Mn_3NiN and Mn_3Ni cases







Mn_3Ni: σ_{xy} = 139 S/cm ($\sigma_{[111]}$ = 241 S/cm)

Mn_3NiN: σ_{xy} = 62 S/cm ($\sigma_{[111]}$ = 107 S/cm)

E. Triana-Ramirez, *et. al.*, Phys. Chem. Chem. Phys. 25, 22, (2023).

Detailed Electronic Structure: Mn_3NiN and Mn_3Ni cases

- Based-on the Born effective charges $Ca_3^{2+}Bi^{3-}N^{3-}$

Chern, M. J. Solid State Chem. 96,415-425.(1992)

- Based-on Mössbauer spectroscopy: $Sr_3^{2+}Sn^{3-}N^{3-}$

Oudah, M et al. Sci. Rep. 9,1-9.(2019)

TABLE III. Effective charges computed by Bader analysis for various antiperovskites A_3BO.

	A = Ca/Sr/Ba	B = Sn/Pb	O
Ca_3SnO	+1.30	−2.38	−1.51
Ca_3PbO	+1.29	−2.35	−1.52
Sr_3SnO	+1.26	−2.30	−1.48
Sr_3PbO	+1.25	−2.26	−1.48
Ba_3SnO	+1.14	−1.98	−1.44
Ba_3PbO	+1.12	−1.93	−1.44

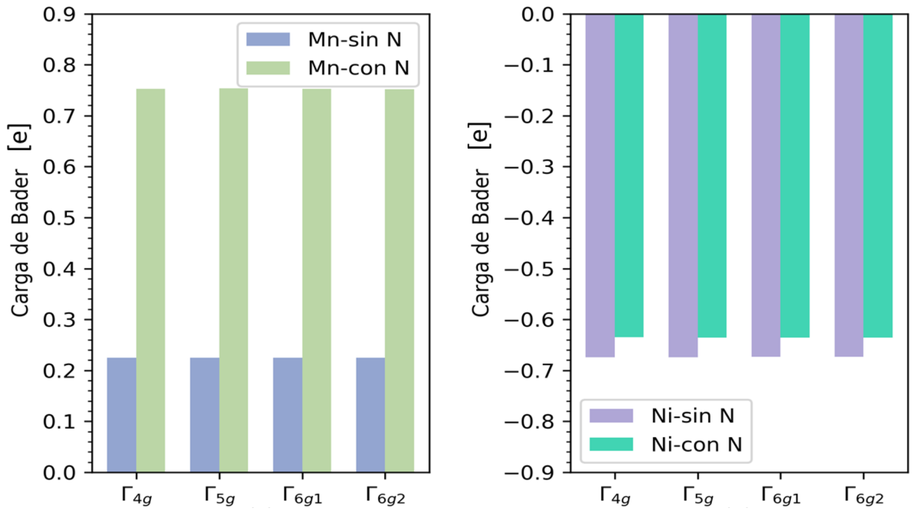
D. Huang. Phys. Rev. Materials 3, 124203 (2019)

- Based-on Mössbauer: $Cs^{1+}Au^{1-}$

Knecht, J et al. J. Chem. Soc. 21,905-906.(1978)

Oxidation State:
The oxidation number in an atom is defined in terms of the charge transfer between atoms.

Walsh, A et at. Nat. Mat 17, 958–964 (2018). Ellis, J. Inorg. Chem. 45, 3167-3186.(2006).

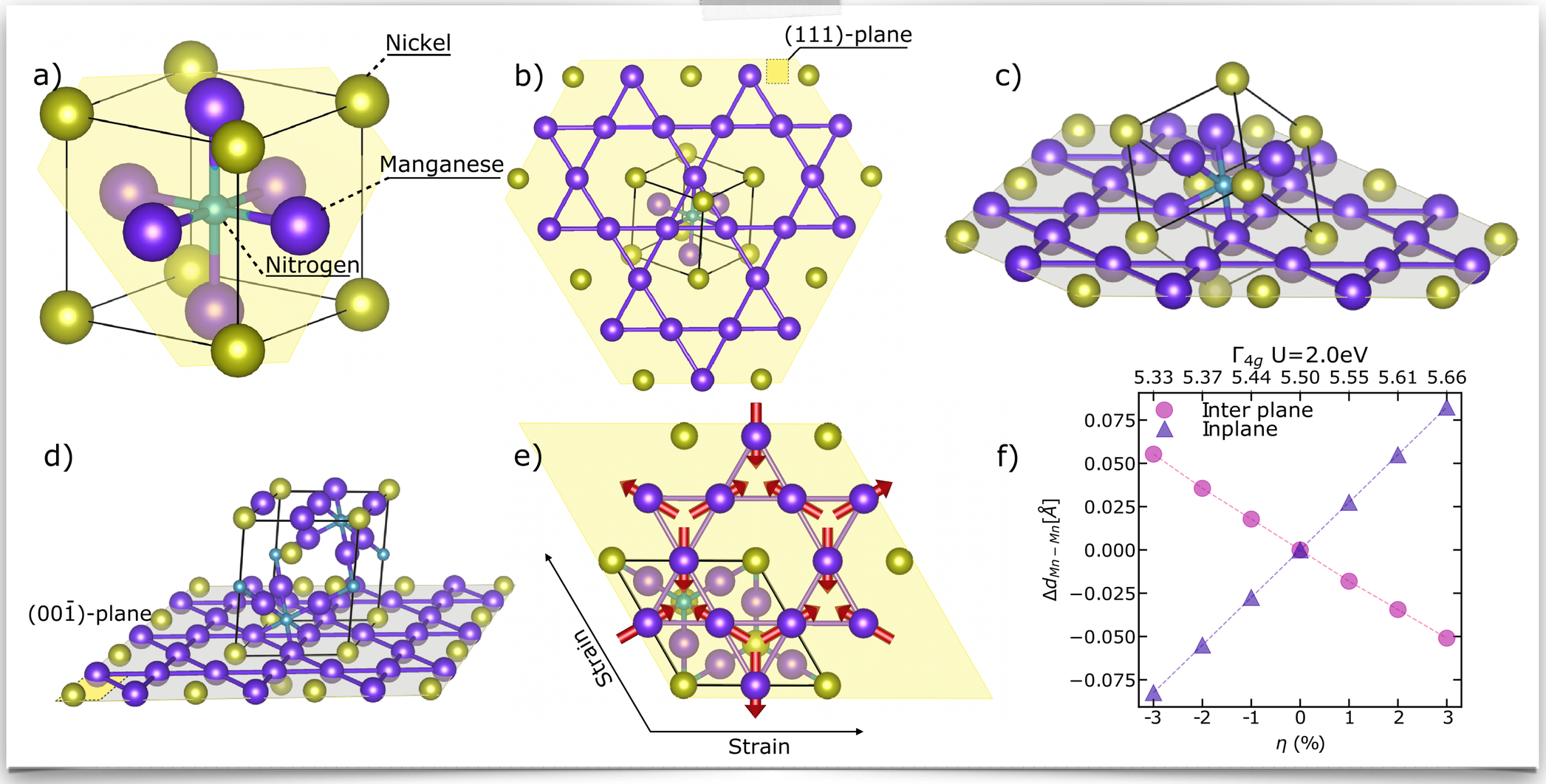


Negative oxidation states in metals…!(?)

E. Triana-Ramirez, *et. al.*, Phys. Chem. Chem. Phys. 25, 22, (2023).

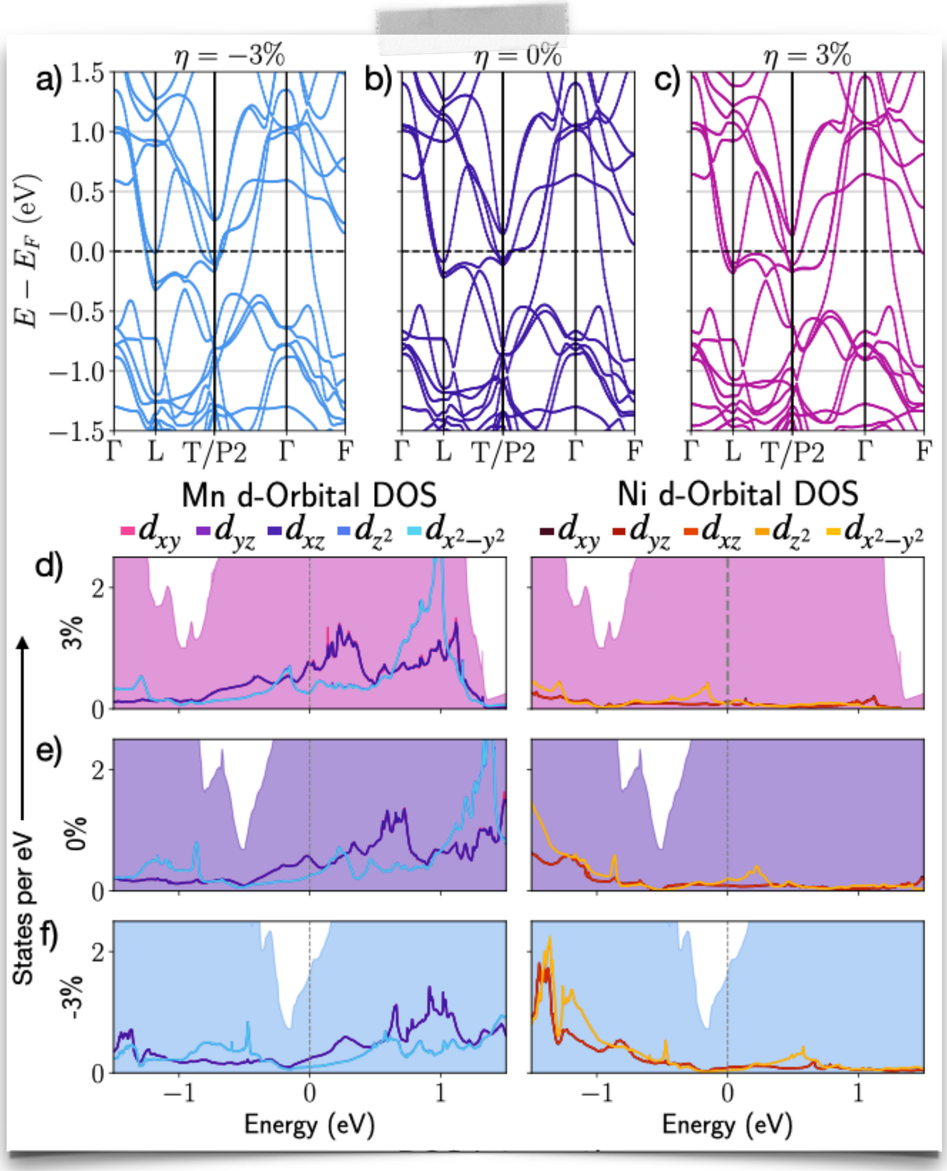
How can we potentially control their electronic properties…?

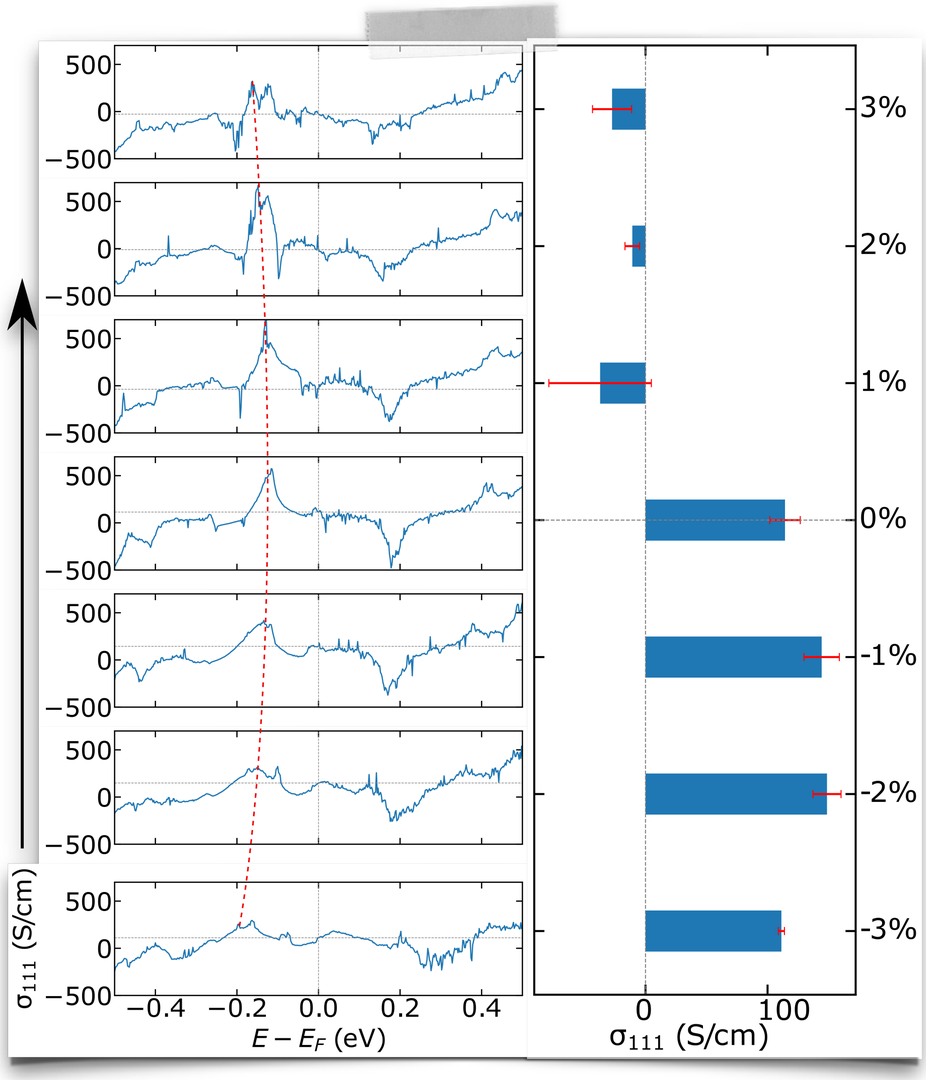
External control: Epitaxial strain effect



D. Torres-Amaris, *et. al.*, Phys. Rev. B. 106, 195113, (2022).

External control: Epitaxial strain effect

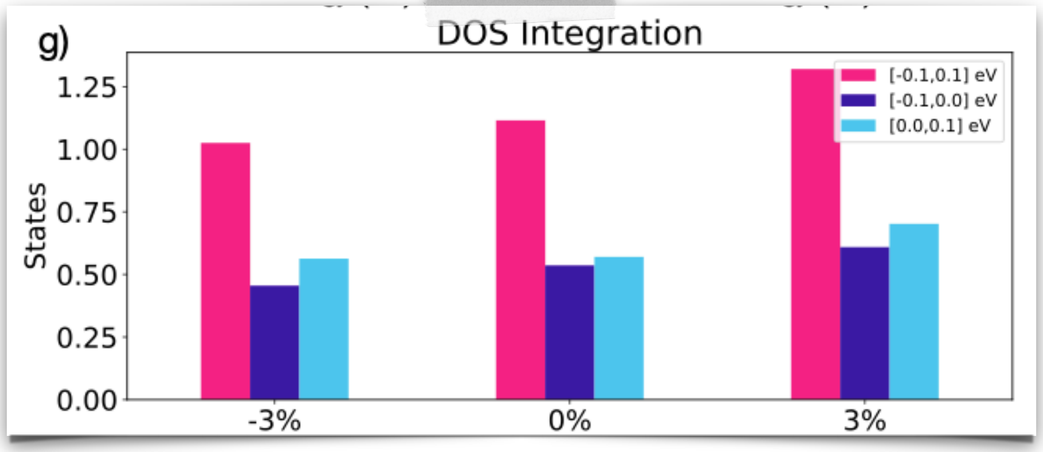


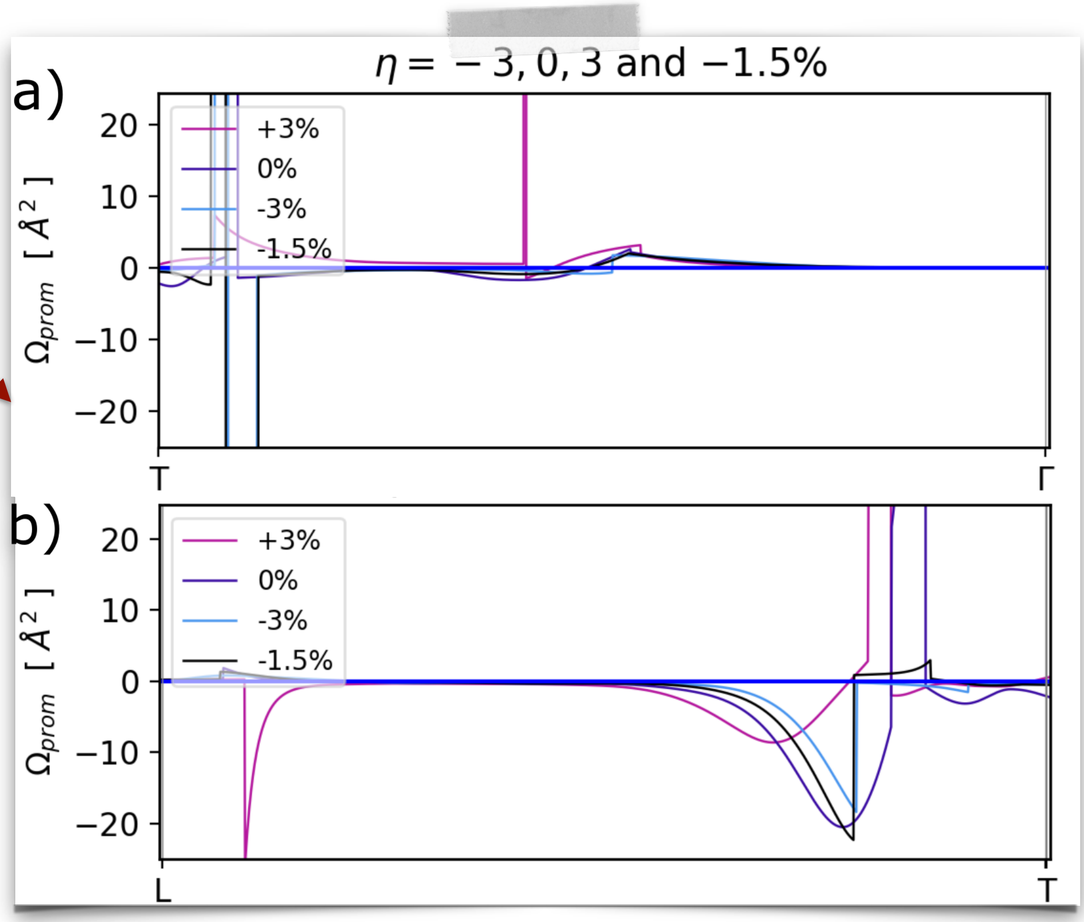


D. Torres-Amaris, *et. al.*, Phys. Rev. B. 106, 195113, (2022).

External control: Epitaxial strain effect

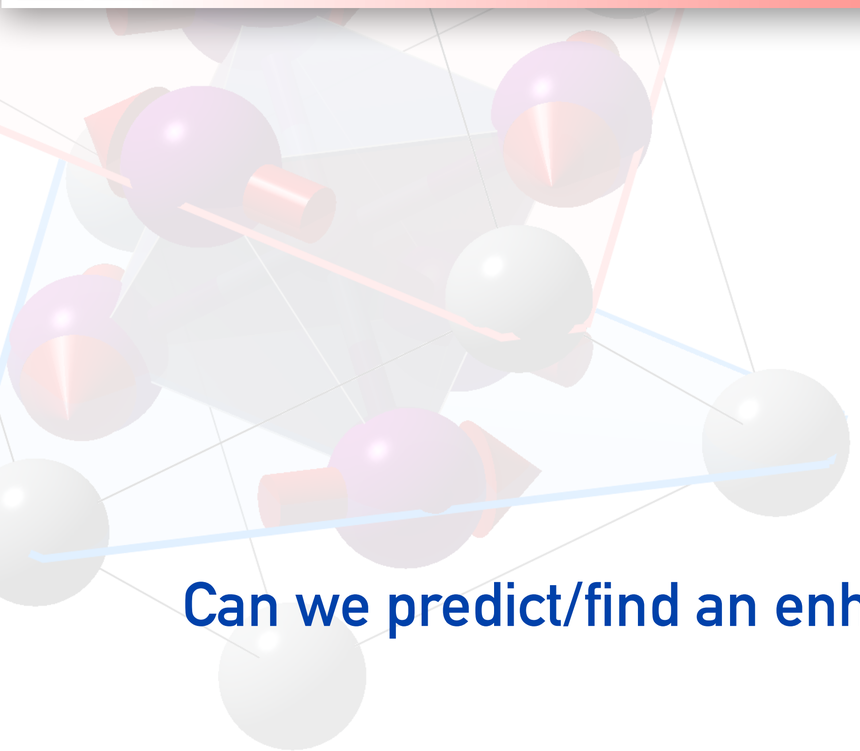
$$\sigma_{\alpha\beta}^{AHC} = -\frac{e^2}{\hbar}\epsilon_{\alpha\beta\gamma}\sum_n \int_{BZ} \frac{d^3\mathbf{k}}{(2\pi)^3} f_n(\mathbf{k})\Omega_n^{\gamma}(\mathbf{k}),$$





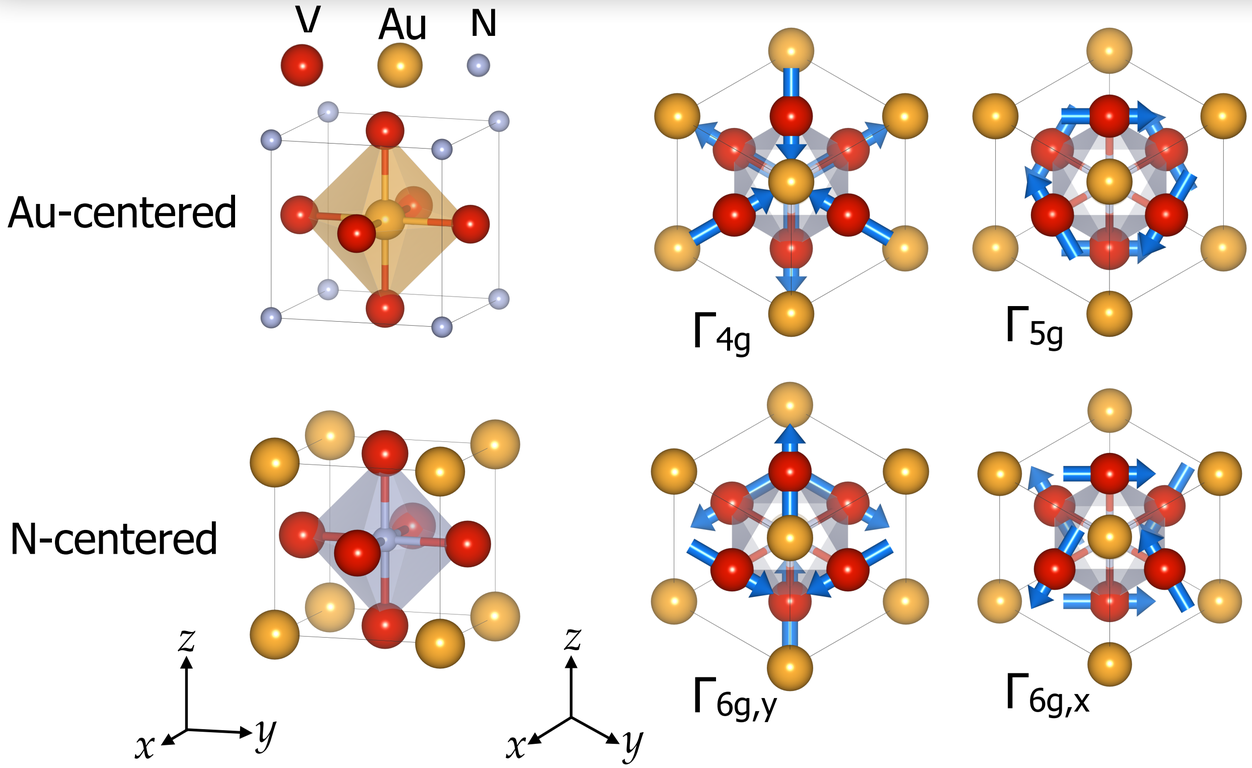
D. Torres-Amaris, *et. al.*, Phys. Rev. B. 106, 195113, (2022).

Novel systems…?



Can we predict/find an enhanced response in novel A_3BN materials…? **Yes…!**

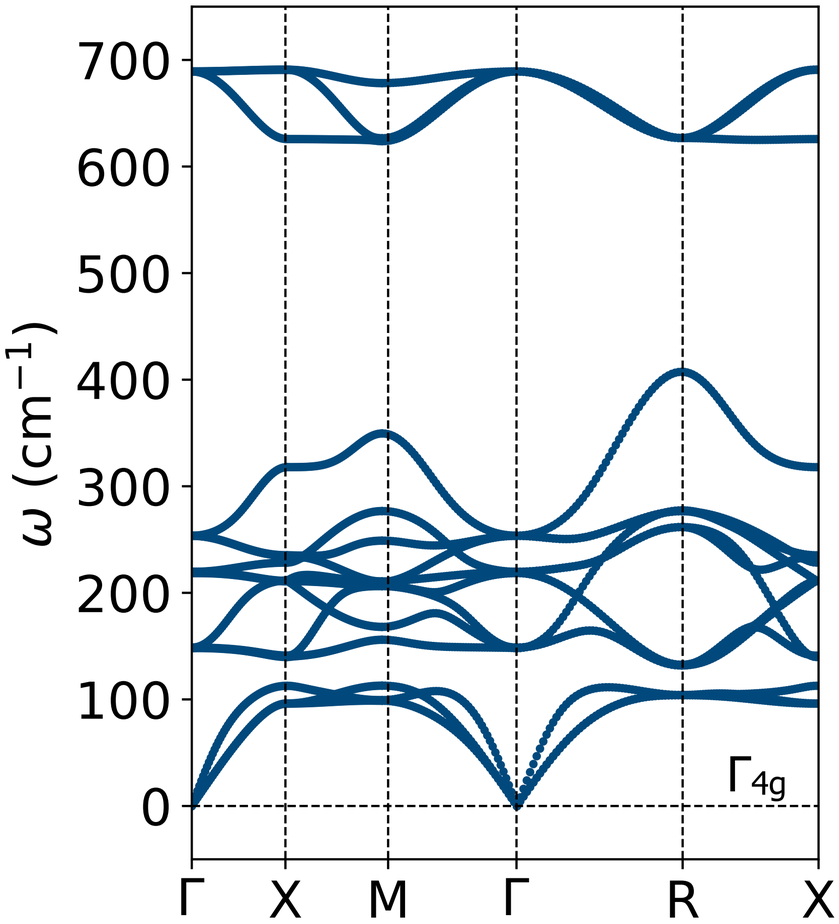
Novel Antiperovskites: The V_3AuN case



W. Rieger, et al., Monatshefte für Chemie und verwandte Teile anderer Wissenschaften 96, 232 (1965).
K. Persson, Materials data on V_3AuN (sg:221) by Materials Project (2016).

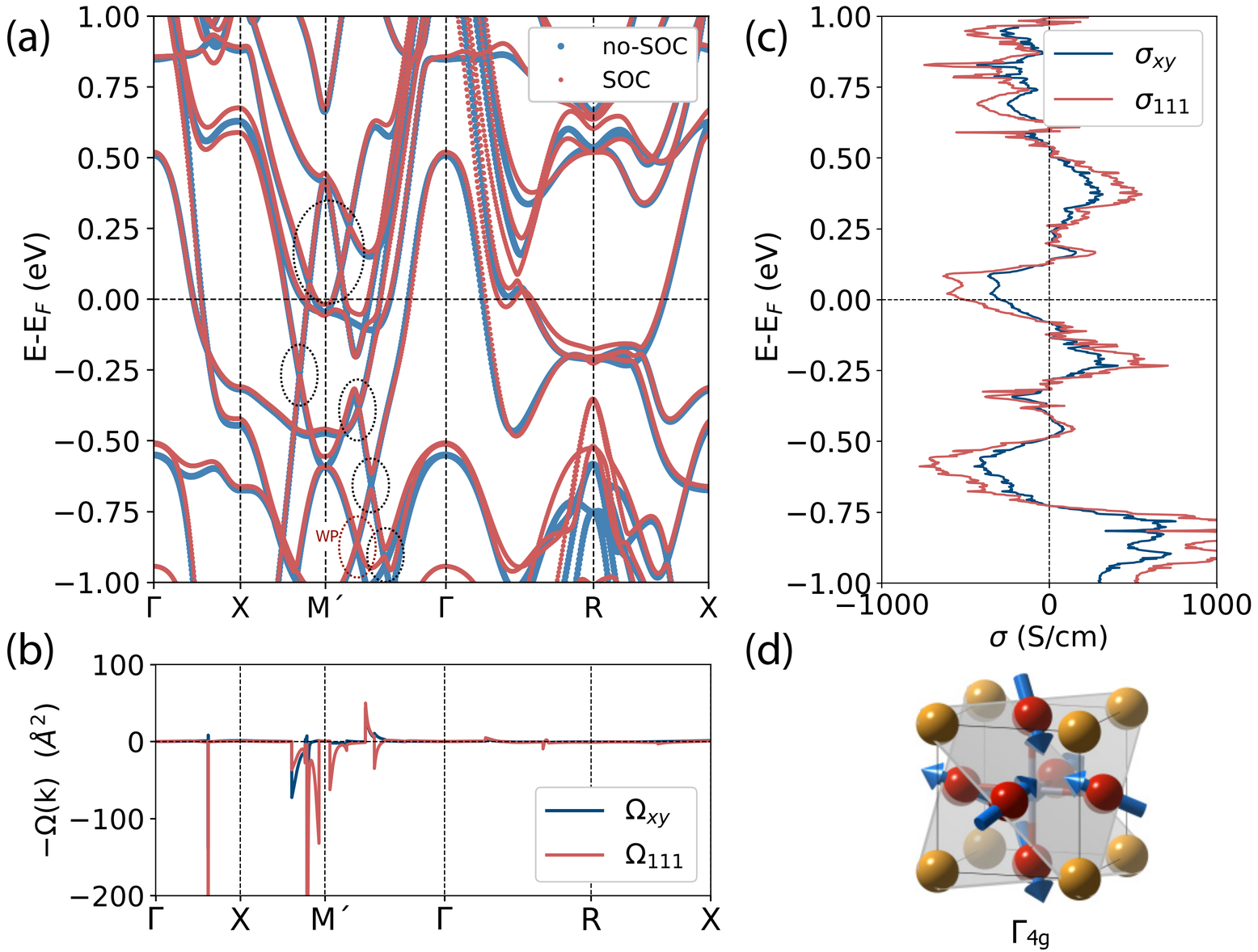
Comp.	$Cmcm$	$Pm\bar{3}m$	ΔE	r_A	t-factor
V_3PN	−44.935	−43.349	+1.586	98	0.84
V_3AsN	−43.275	−42.416	+0.860	114	0.89
V_3SbN[a]	−41.603	−41.506	+0.097	133	0.95
V_3AuN	−41.362	−41.562	−0.200	174	1.07

B. Wang, K. Ohgushi, Sci. Rep. 2013, 3, 3381.
M. Oudah, et al. Nat. Commun. 2016, 7, 13617
A. C. Garcia-Castro, et al., Phys. Rev. B 90, 064113 (2014).



J.M. Duran-Pinilla *et. al.*, Phys. Rev. Mat. 6,125003, (2022).

Novel Antiperovskites: The V_3AuN case



V_3AuN (PBEsol+U)

σ_{xy} = 435 S/cm

σ_{111} = 753 S/cm

Mn_3PtN (PBE)

σ_{xy} = 462 S/cm

σ_{111} = 800 S/cm

Vu Thi Ngoc Huyen, et al. Phys. Rev. B, 100, 094426 (2019).

Mn_3PtN (PBEsol+U)

σ_{xy} = 144 S/cm

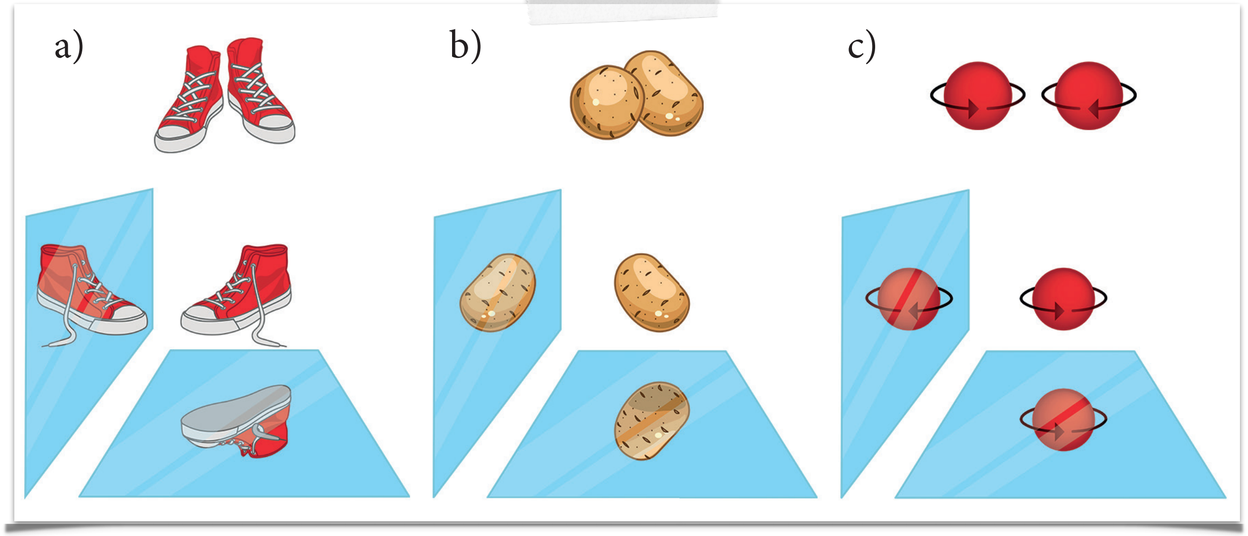
σ_{111} = 249 S/cm

J.M. Duran-Pinilla *et. al.*, Phys. Rev. Mat. 6,125003, (2022).

Chirality in Crystals?

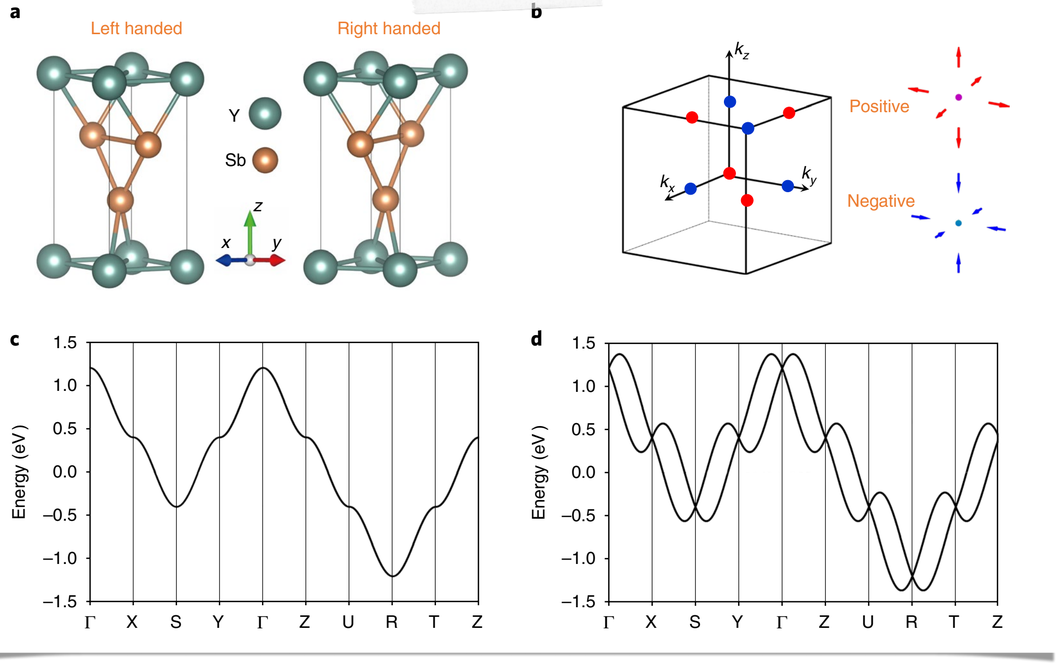
What happens with the chiral symmetry in the crystallography…?

Chirality in crystals…

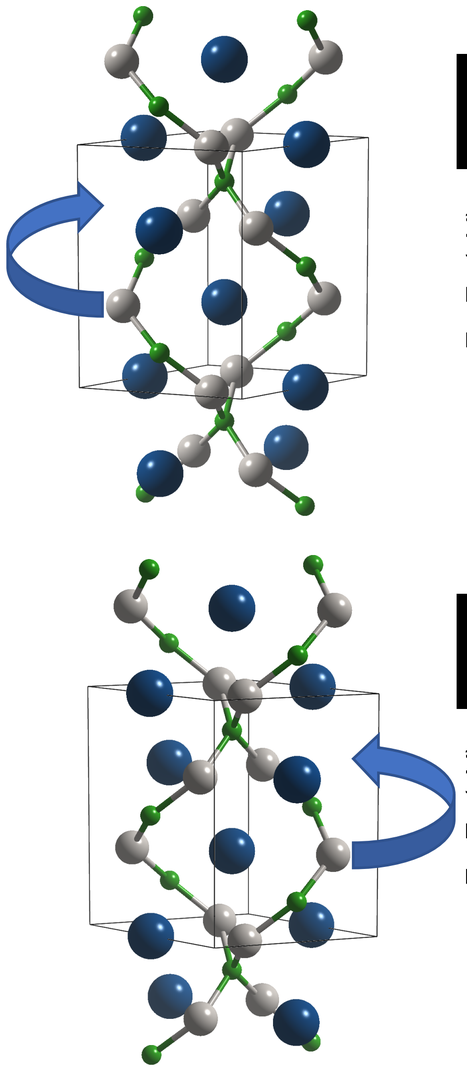


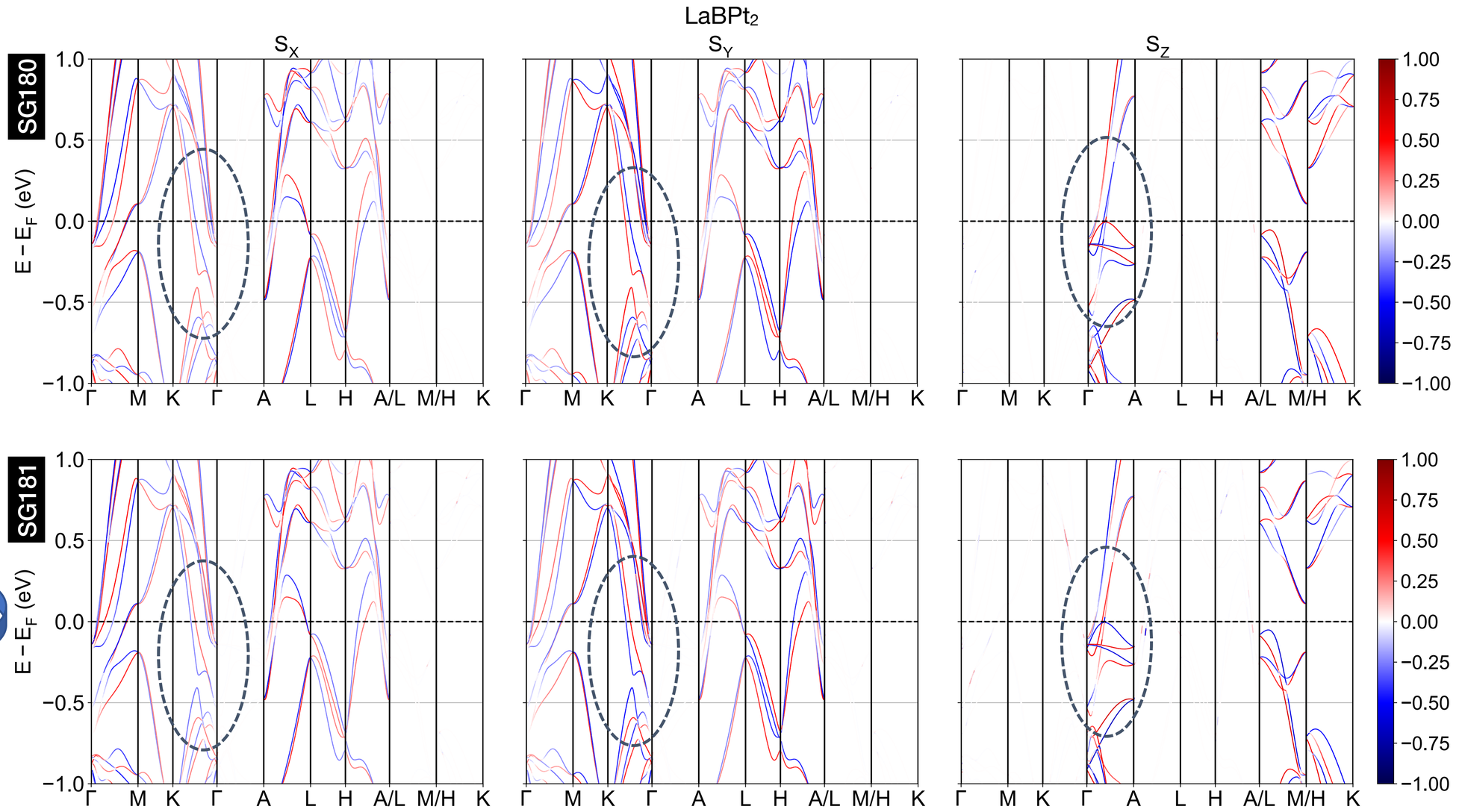
Gerhard Fecher et. al., Materials, 15(17), 5812 (2022).

Guoqing Chang et. al., Nature Materials, 17, 978–985 (2018).



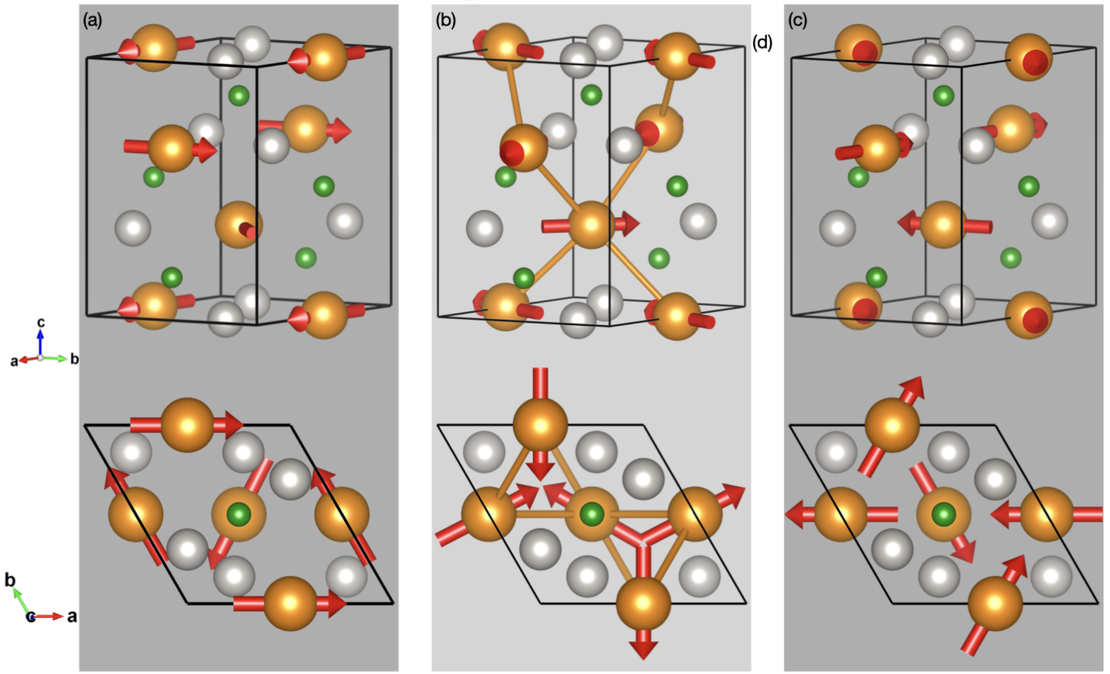
Novel systems…

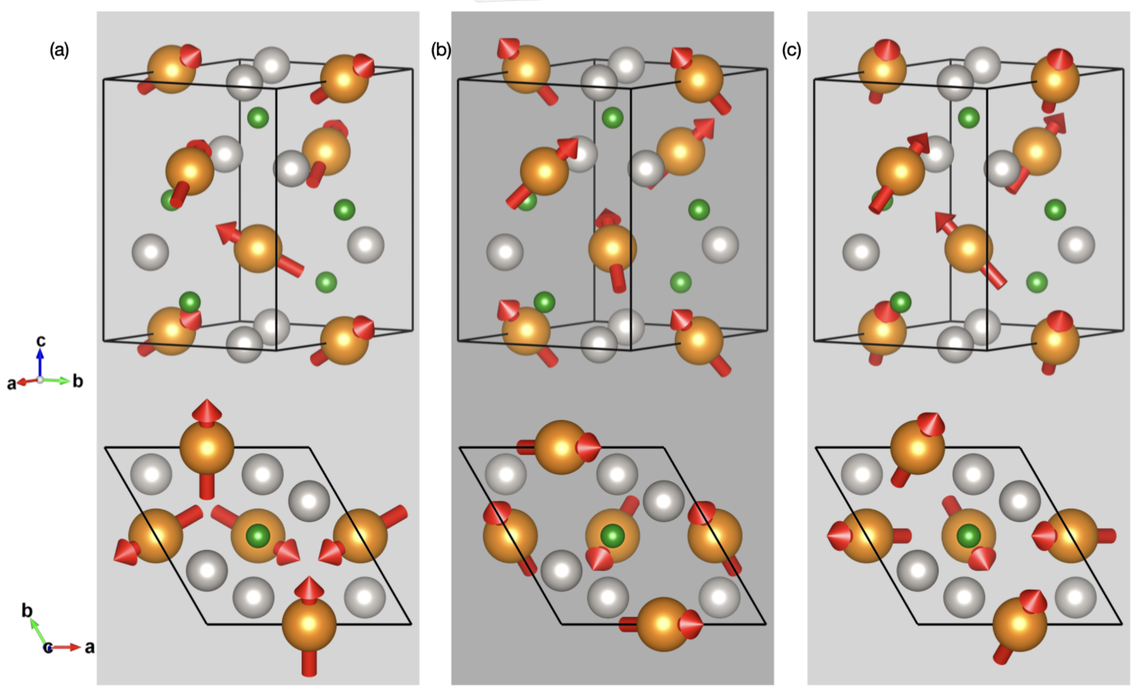




D. Torres-Amaris *et. al.*, Phys. Rev. B. To be Submitted (2023).

Novel systems…





D. Torres-Amaris *et. al.*, Phys. Rev. B. To be Submitted (2023).

General remarks…!

✓ *Strong spin-phonon coupling in Mn_3NiN antiferromagnetic antiperovskite*

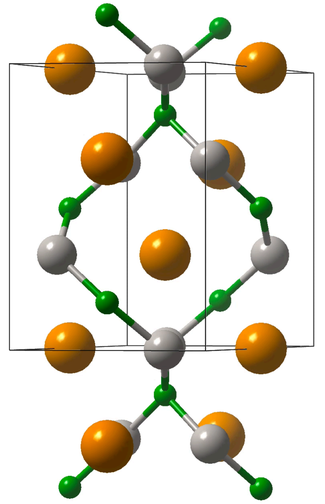
✓ *Large influence of the exchange-correlation effects*

✓ *Strain control of the topologically-related electronic properties*

✓ *Prediction of the novel and enhanced antiperovskite compound*

What is next…?

Chiral symmetry+chiral magnetism!



Thank you for your attention! Questions?

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