

# Multifunctional properties induced by chirality in crystalline materials

(Characterization of  $Mn_3PtN$ )

Daniel D. Torres

Doctorado en Física

Adv. Iliia D. Mikhailov PhD CoAdv. Andrés C. García PhD

Grupo de Física Computacional y Materia Condensada

Facultad de Ciencias

Escuela de Física

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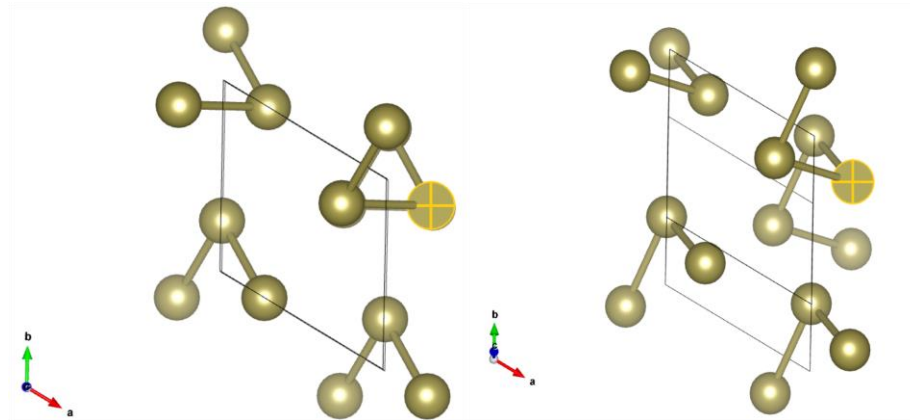
# What's Chirality?



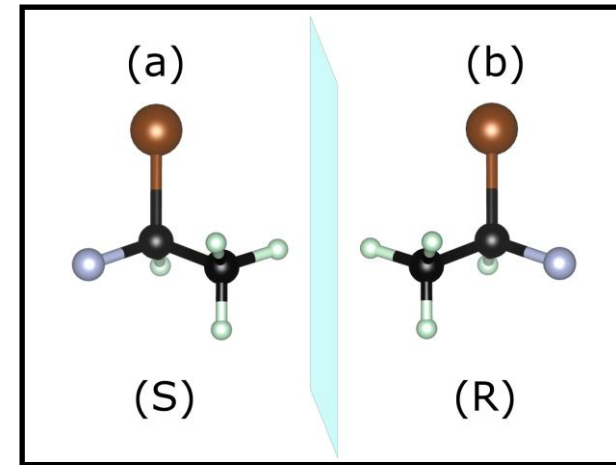
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Everyday objects  
can be chiral



There is chirality in crystals



Chirality in molecules

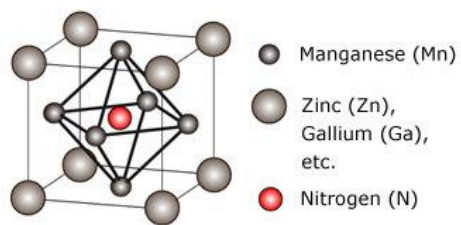


# The $Mn_3AN$ antiperovskites

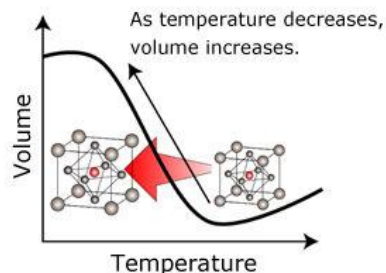
## Magnetic frustration



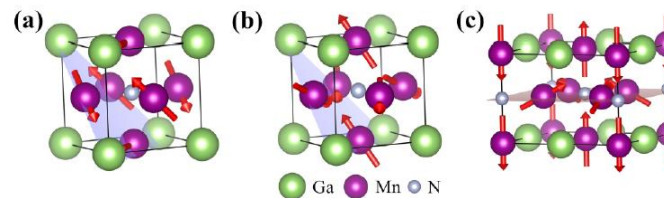
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**Fig.1:** Crystal structure of inverse perovskite antiferromagnets  $Mn_3AN$  ( $A = Zn, Ga, \text{etc.}$ ).



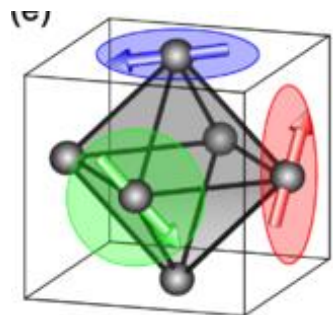
**Fig.2:** Concept of negative thermal expansion (or NTE).



**FIG. 1.** Different noncollinear magnetic phases in AFM antiperovskite  $GaNm_3$ : (a)  $\Gamma_{5g}$ , (b)  $\Gamma_{4g}$ , and (c) M-1. Red arrows denote magnetic moments.

**TABLE II.** Calculated lattice parameters  $a$  and AHC  $\sigma_{xy}$  for different magnetic phases of  $ANm_3$  ( $A = Ga, Ni, Sn$ ).

$ANm_3$	$a(\text{\AA})$			$\sigma_{xy} (\Omega^{-1} \text{cm}^{-1})$		
	$\Gamma_{5g}$	$\Gamma_{4g}$	M-1	$\Gamma_{5g}$	$\Gamma_{4g}$	M-1
$GaNm_3$	3.87	3.87	3.82	0	40	377
$NiNm_3$	3.84	3.84		0	130	
$SnNm_3$	3.99	3.99		0	133	



PHYSICAL REVIEW MATERIALS 3, 024407 (2019)

### Theory of magnetism-driven negative thermal expansion in inverse perovskite antiferromagnets

Masaya Kobayashi<sup>1</sup> and Masahito Mochizuki<sup>1,2</sup>

<sup>1</sup>Department of Physics and Mathematics, Aoyama Gakuin University, Sagamihara, Kanagawa 229-8558, Japan

<sup>2</sup>Department of Applied Physics, Waseda University, Okubo, Shinjuku-ku, Tokyo 169-8555, Japan

PHYSICAL REVIEW MATERIALS 3, 044409 (2019)

### Anomalous Hall conductivity of noncollinear magnetic antiperovskites

Gautam Gurung, Ding-Fu Shao,<sup>\*</sup> Tula R. Paudel, and Evgeny Y. Tsymbal<sup>†</sup>

Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, Nebraska 68588-0299, USA

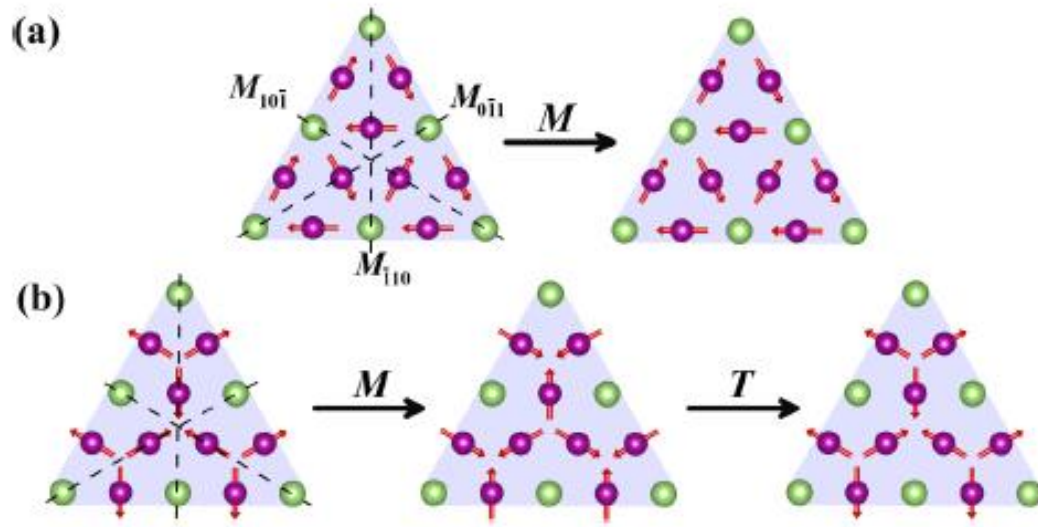
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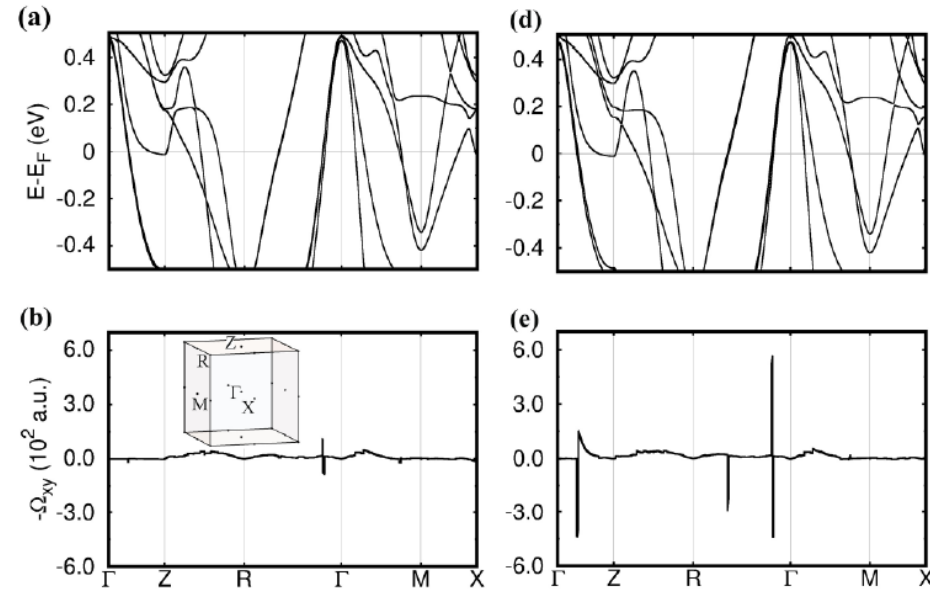


# The $Mn_3AN$ antiperovskites

## Magnetic phases and properties



(a)  $\Gamma_{5g}$  (b)  $\Gamma_{4g}$  magnetic orderings band structures and their symmetry operations



(a)  $\Gamma_{5g}$  (b)  $\Gamma_{4g}$  magnetic orderings band structures and their corresponding berry curvatures in (b) and (c)

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### Anomalous Hall conductivity of noncollinear magnetic antiperovskites

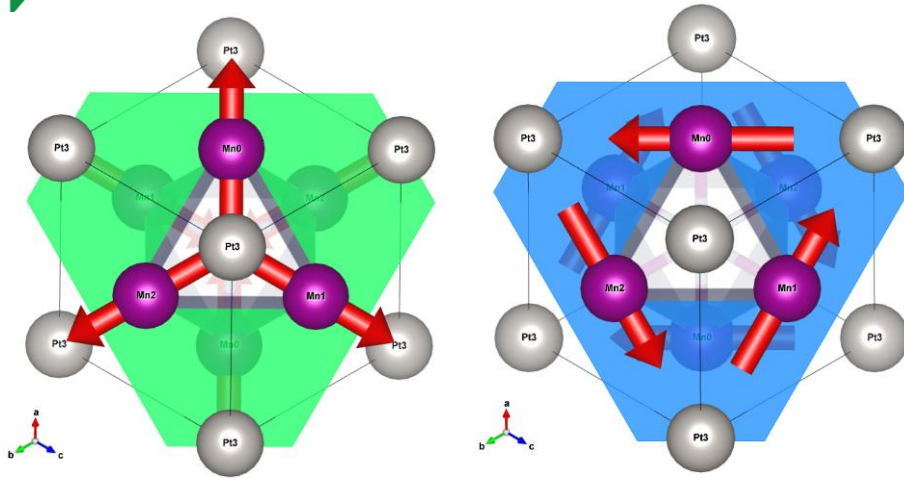
Gautam Gurgung, Ding-Fu Shao,\* Tula R. Paudel, and Evgeny Y. Tsymbal†  
Department of Physics and Astronomy and Nebraska Center for Materials and Nanoscience, University of Nebraska,  
Lincoln, Nebraska 68588-0299, USA

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# Characterization of $Mn_3PtN$

Ionic and electronic optimization



$\Gamma_{5g}$  and  $\Gamma_{4g}$  magnetic ordering in  $Mn_3PtN$

Both structures are stable

After the optimization, we found the lattice parameter  $a = 3.973\text{\AA}$ . The value reported according to experimental characterization is  $a=3.969\text{\AA}$ .

Structure, magnetic properties and thermal expansion of  $Mn_3PtN_x$  ( $0 \leq x \leq 1.0$ ) compounds

Ruihua Chou

*The High School Affiliated to Renmin University of China,  
Beijing 100080, P. R. China*

Ying Sun\*, Huiqing Lu and Guang-Hong Lu

*Department of Physics,  
Beihang University, Beijing 100191, P. R. China*

*\*sunying@buaa.edu.cn*

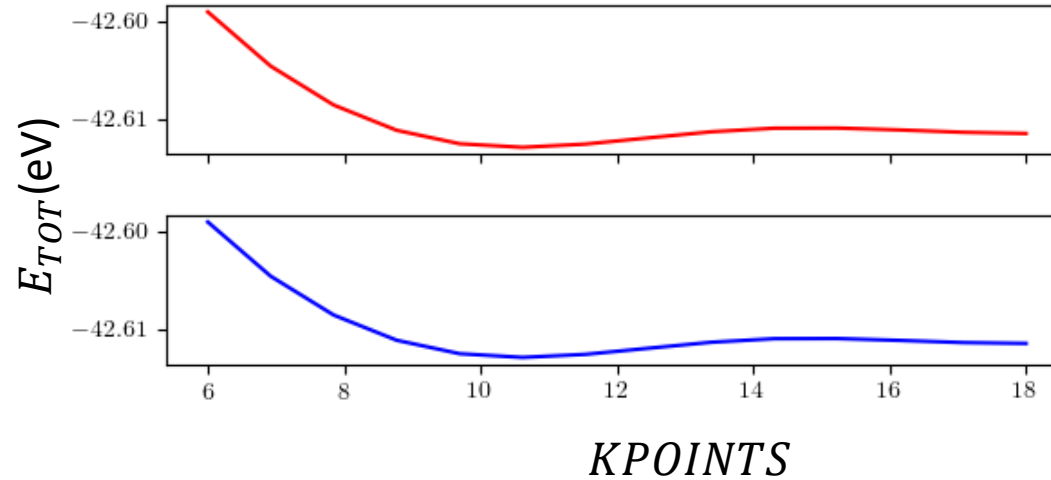
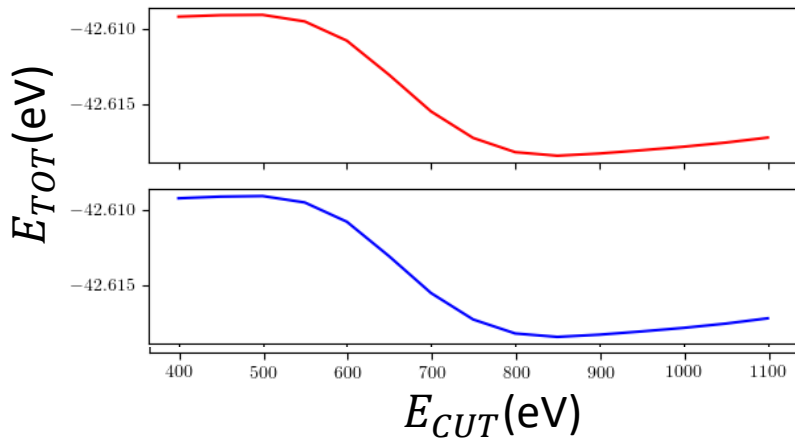


# Characterization of $Mn_3PtN$

Convergence study



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We aimed for meV precision



We selected  $E_{CUT} = 800eV$  and 12 KPOINTS

JOURNAL OF APPLIED PHYSICS 108, 113920 (2010)

Nature of the negative thermal expansion in antiperovskite compound  $Mn_3ZnN$

B. Y. Qu and B. C. Pan<sup>a)</sup>  
Department of Physics, Hefei National Laboratory for Physical Sciences at Microscale, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

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# Characterization of $Mn_3PtN$

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



Bands + DOS

High AHC →

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,<sup>1,2,3</sup> Michi-To Suzuki<sup>4,\*</sup>, Kunihiro Yamauchi,<sup>1</sup> and Tamio Oguchi<sup>1,2</sup>

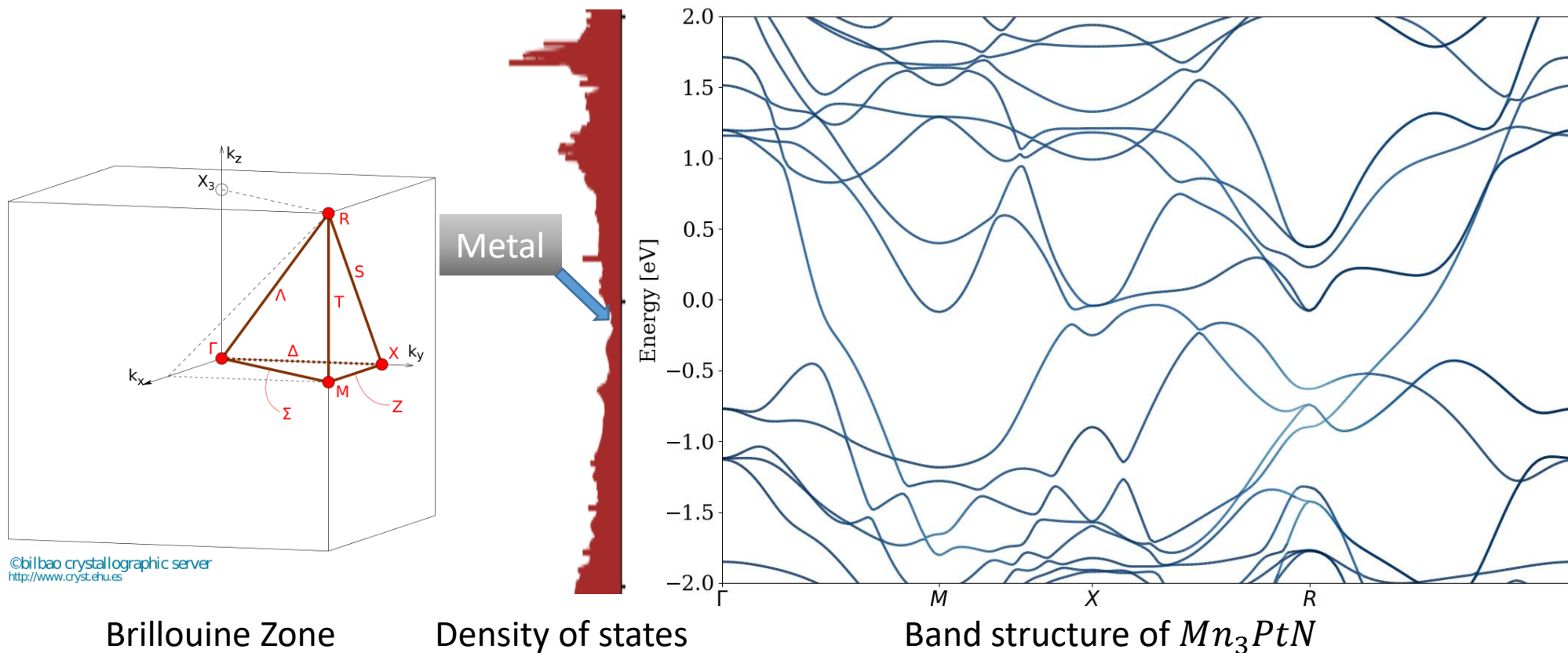
<sup>1</sup>Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, Osaka 567-0047, Japan

<sup>2</sup>Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan

<sup>3</sup>Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

<sup>4</sup>Center for Computational Materials Science, Institute for Materials Research, Tohoku University, Sendai, Miyagi 980-8577, Japan

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Brillouine Zone

Density of states

Band structure of  $Mn_3PtN$

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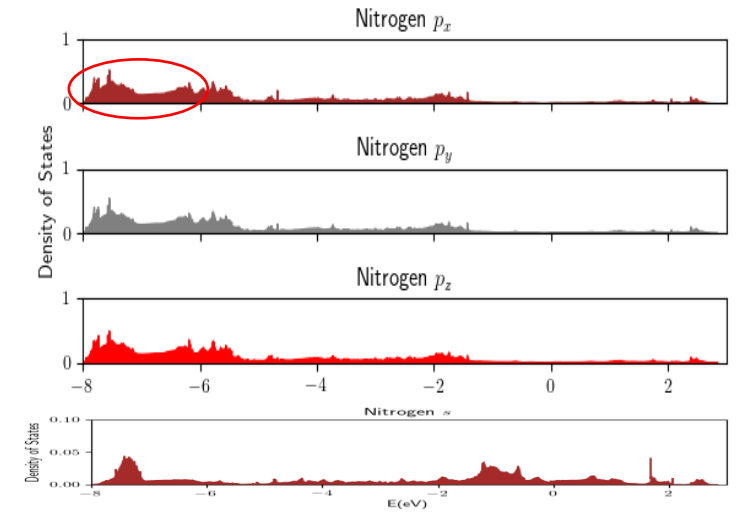
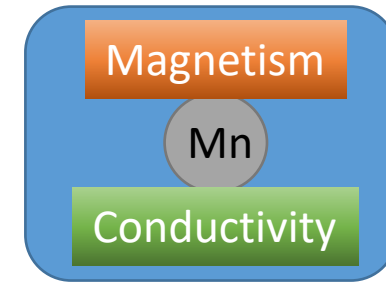
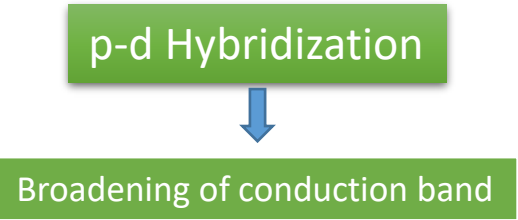
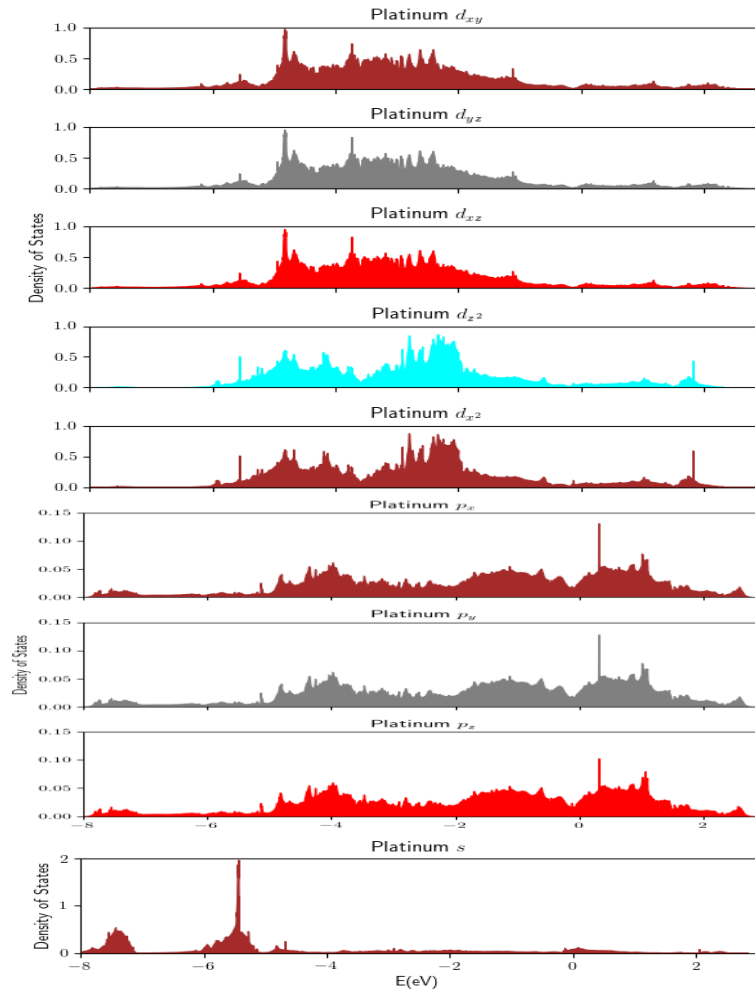
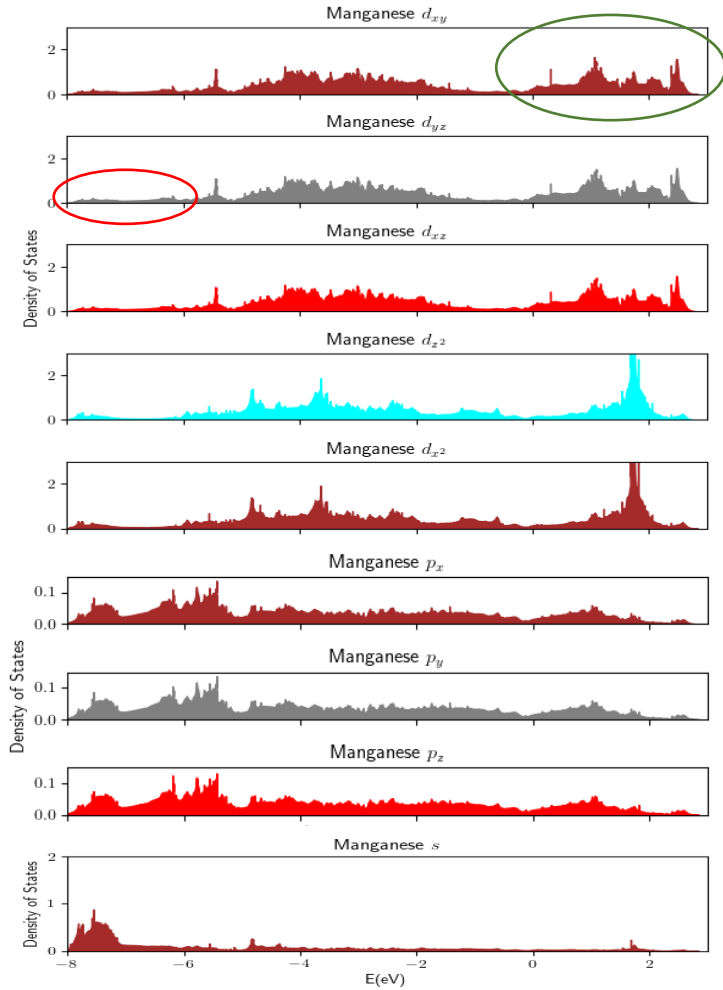




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# Characterization of $Mn_3PtN$

## Partial DOS



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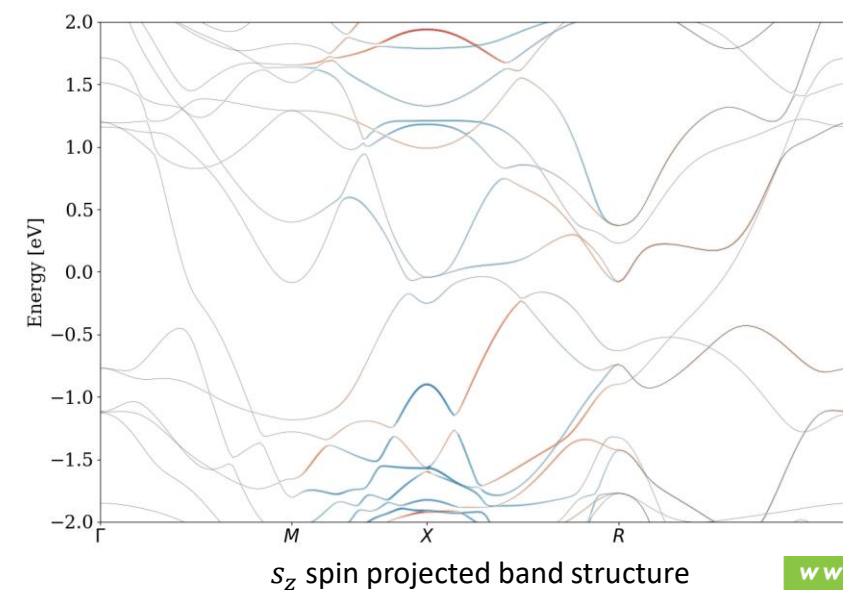
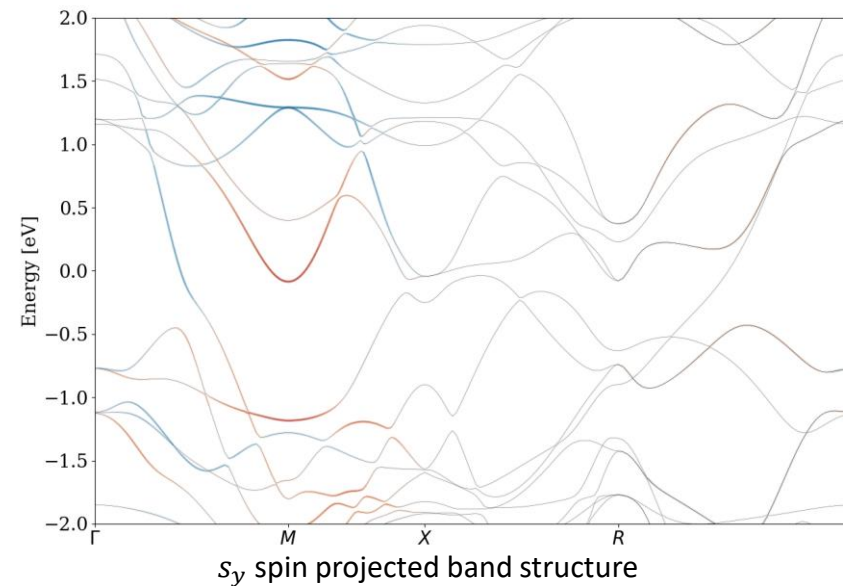
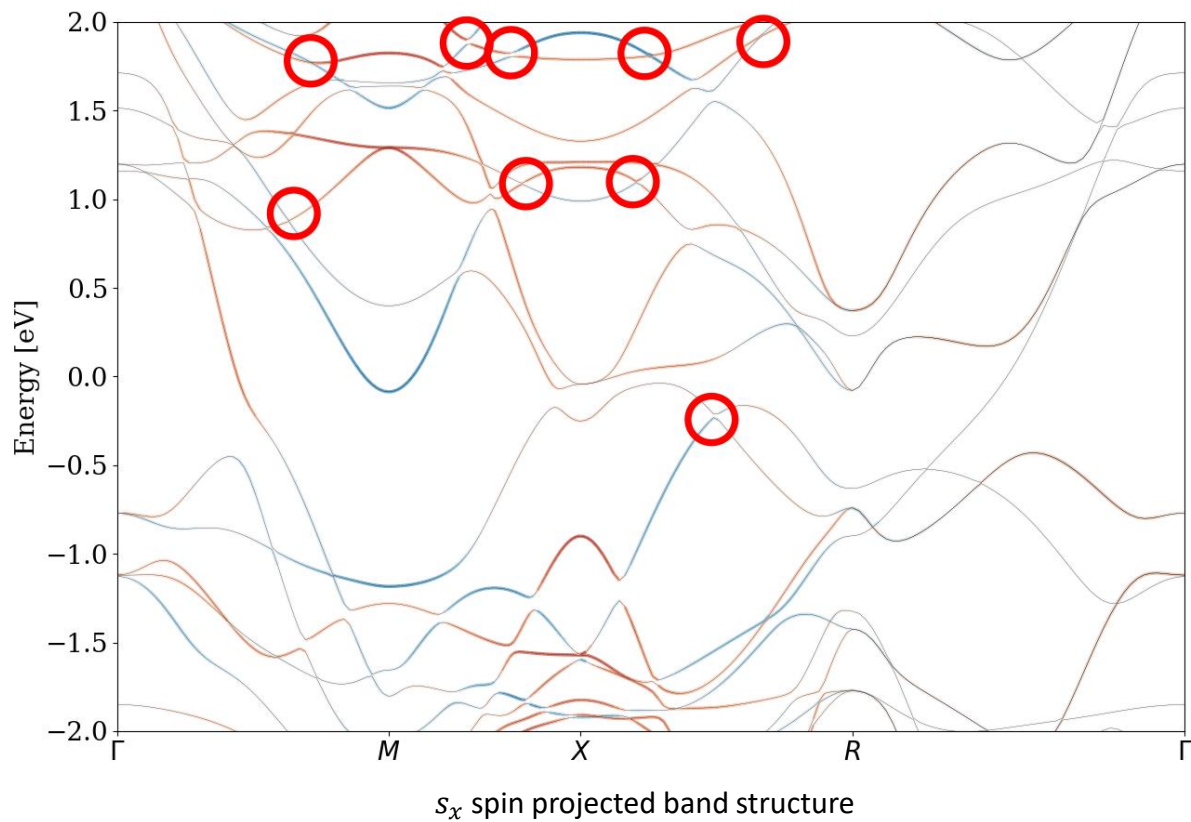


# Characterization of $Mn_3PtN$

Weyl Points



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