DFT+DMFT for honeycomb lattices in (111) oxide heterostructures

Oleg Janson

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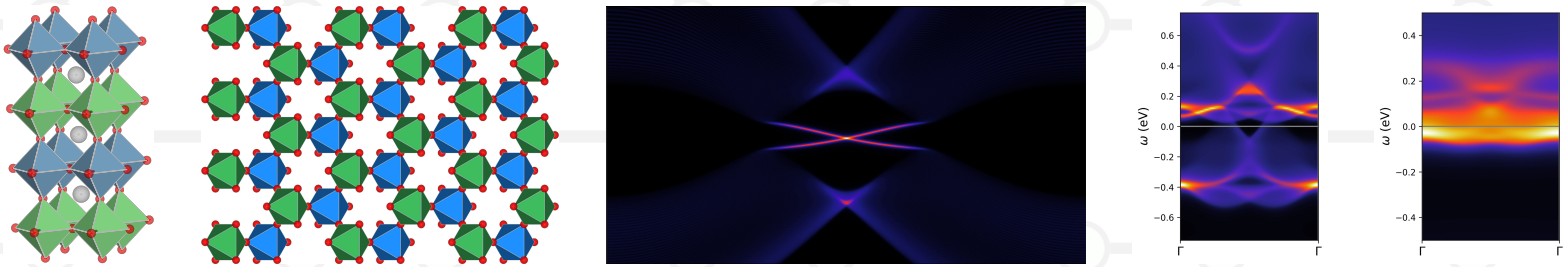
Dresden



UKRATOP Workshop “Topological Phenomena in Quantum Materials”
Dresden, 05.12.2018

Outline

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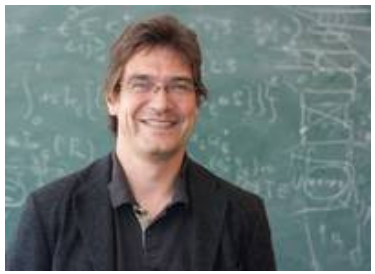
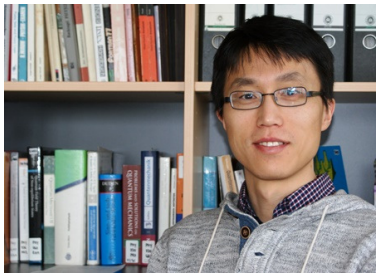
Acknowledgements



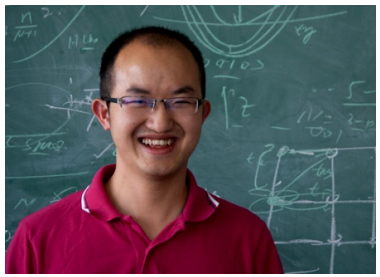
Karsten Held

Liang Si

TU WIEN



Gang Li
(now at ShanghaiTech)

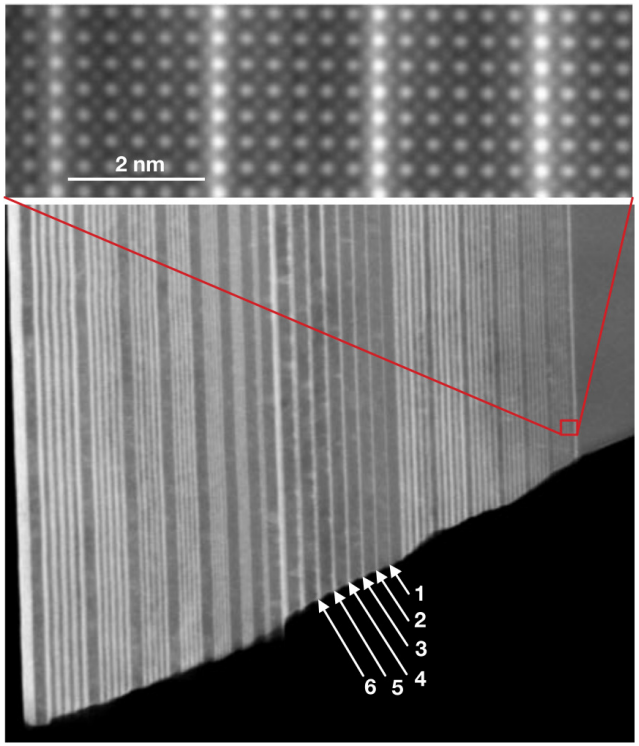


Zhicheng Zhong
(now at CNITECH, CAS)

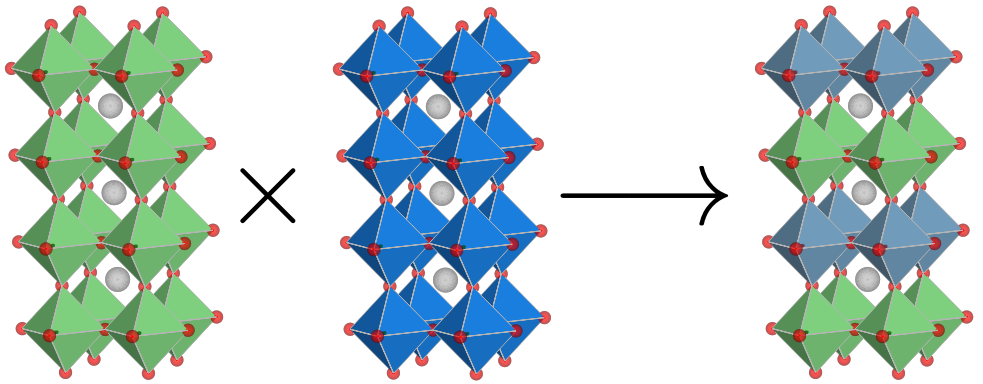
FWF Der Wissenschaftsfonds.

Lise Meitner Programme, M2050

Oxide heterostructures based on the perovskite structure

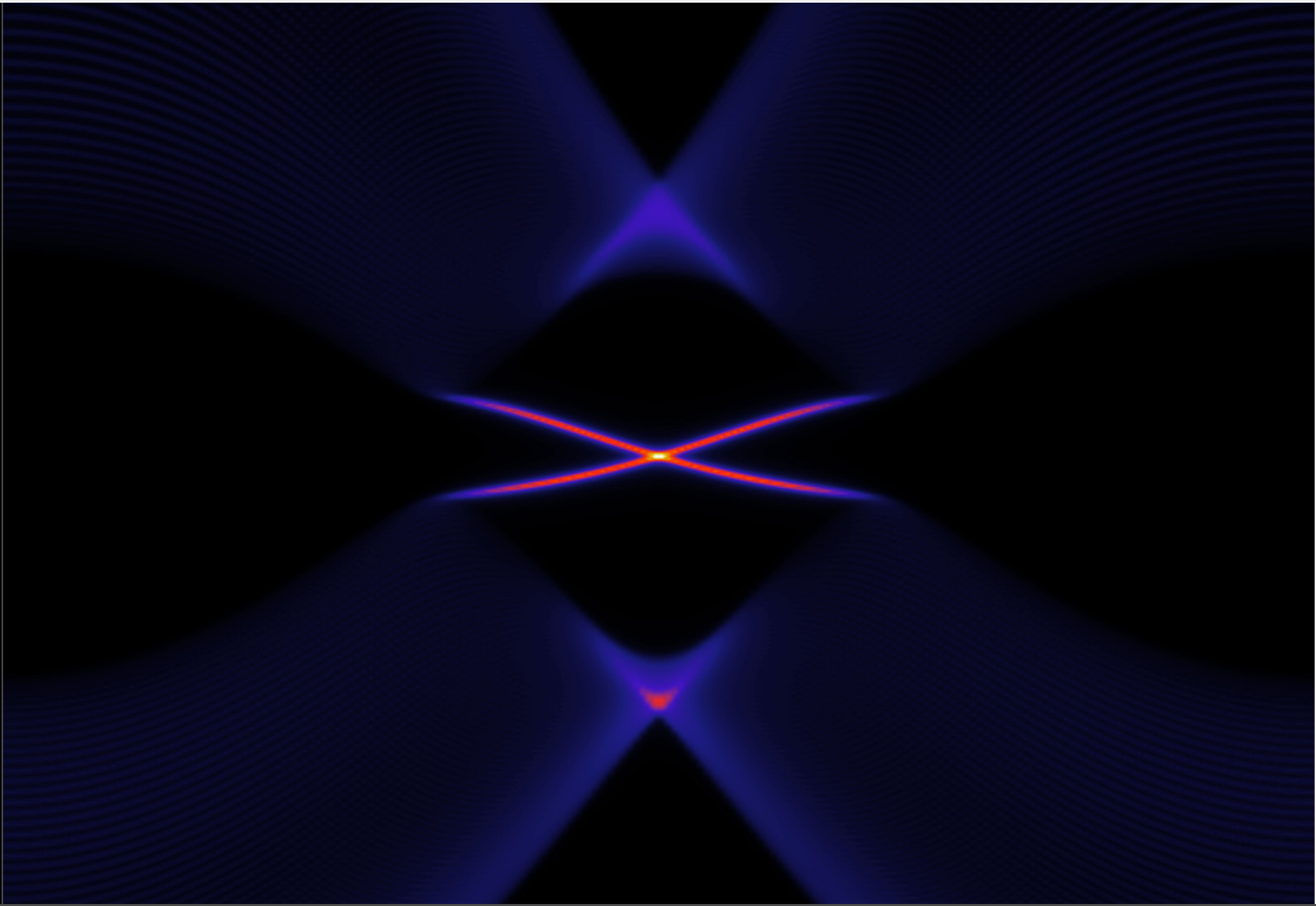


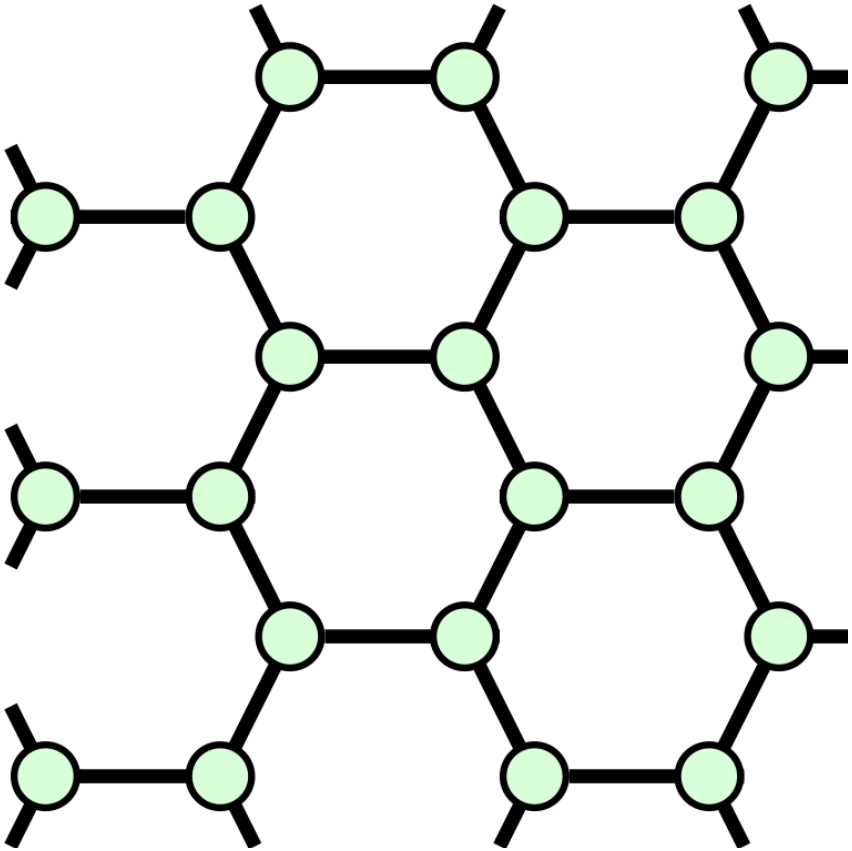
A. Ohtomo *et al.*, Nature **419**, 378 (2002)



2D electron gas at the interfrace between $LaAlO_3$ (insulator) and $SrTiO_3$ (insulator)

chemical flexibility $\rightarrow$ tunable physics?

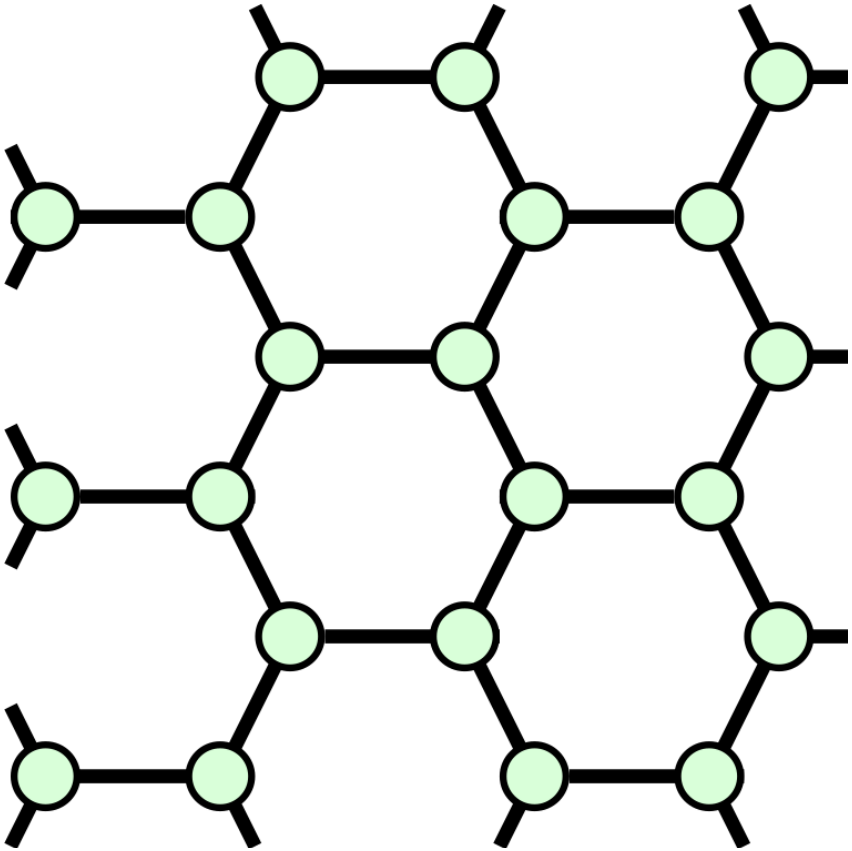




graphene

Excellent QSH system, but

- SOC too small
- nonlocal interactions (~~Hubbard model~~)



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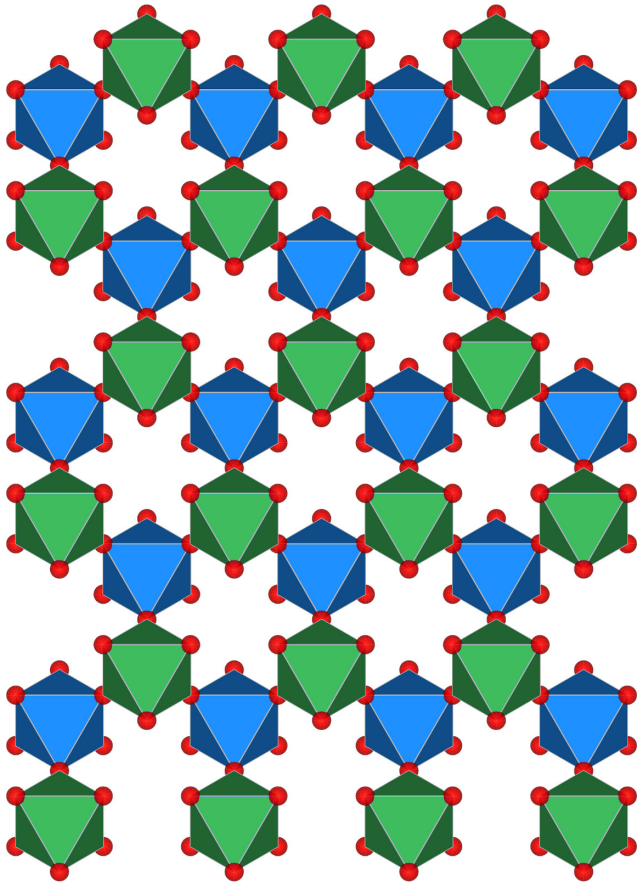
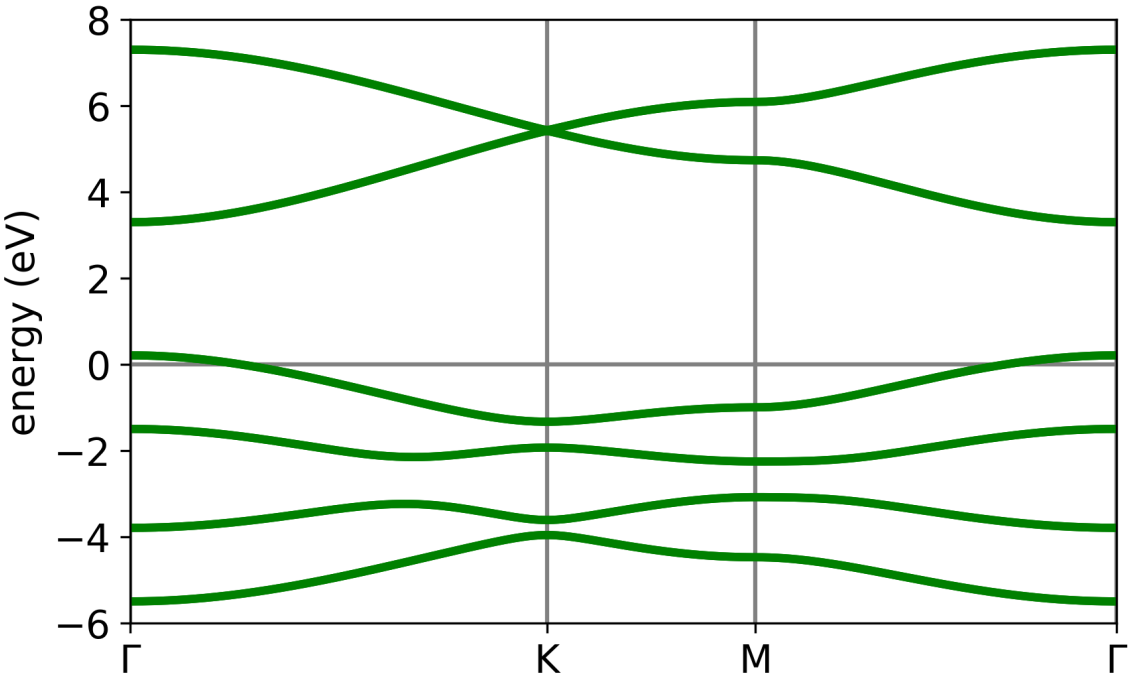


(111) perovskite bilayers

- flexible U, J, and SOC
- heterostructures can be grown

correlated analogs of graphene
$\rightarrow$ topology?

TB model for *d* electrons on a honeycomb lattice: D. Xiao *et al.*, Nat. Comm. **2**, 596 (2011)
TI (QSH) and Chern insulators (QAH) can be stabilized at different fillings



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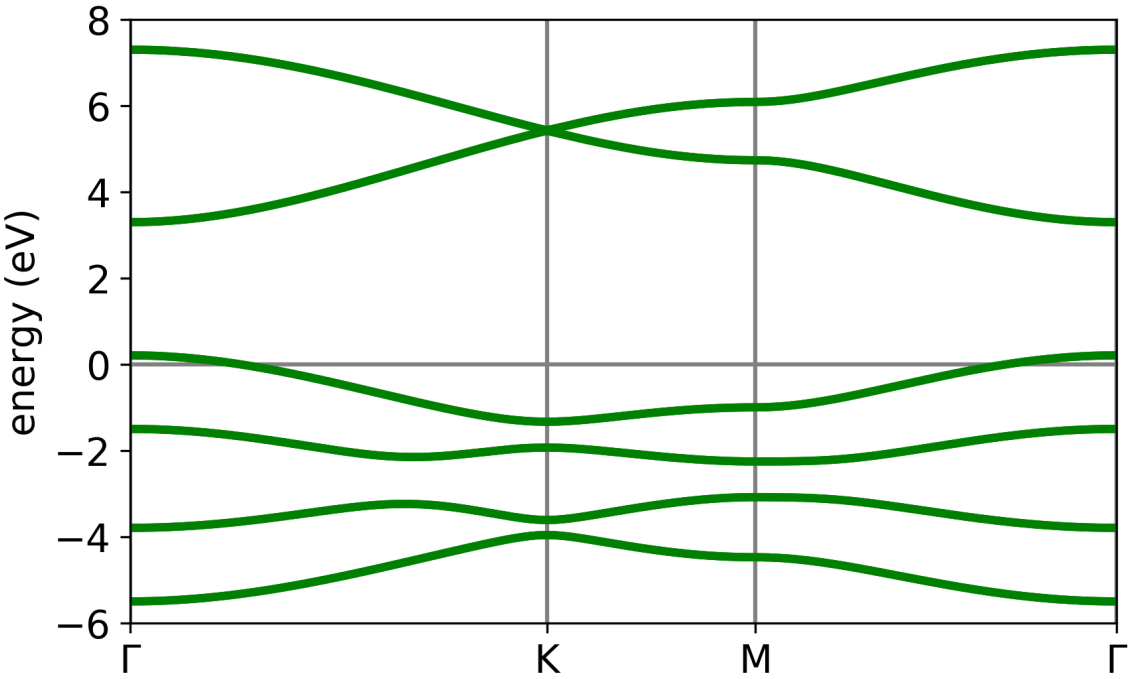

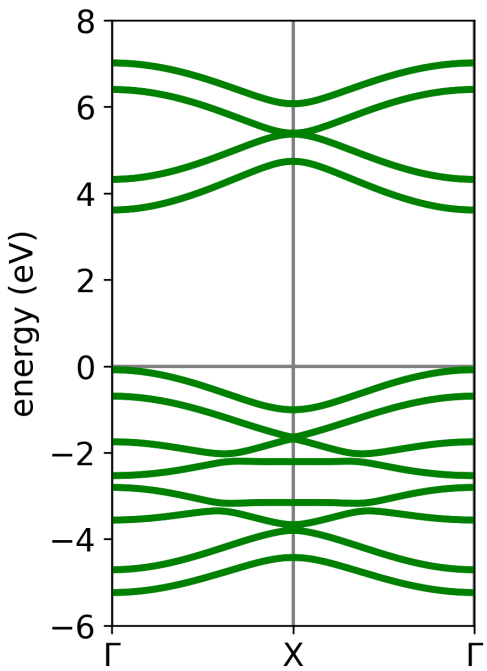

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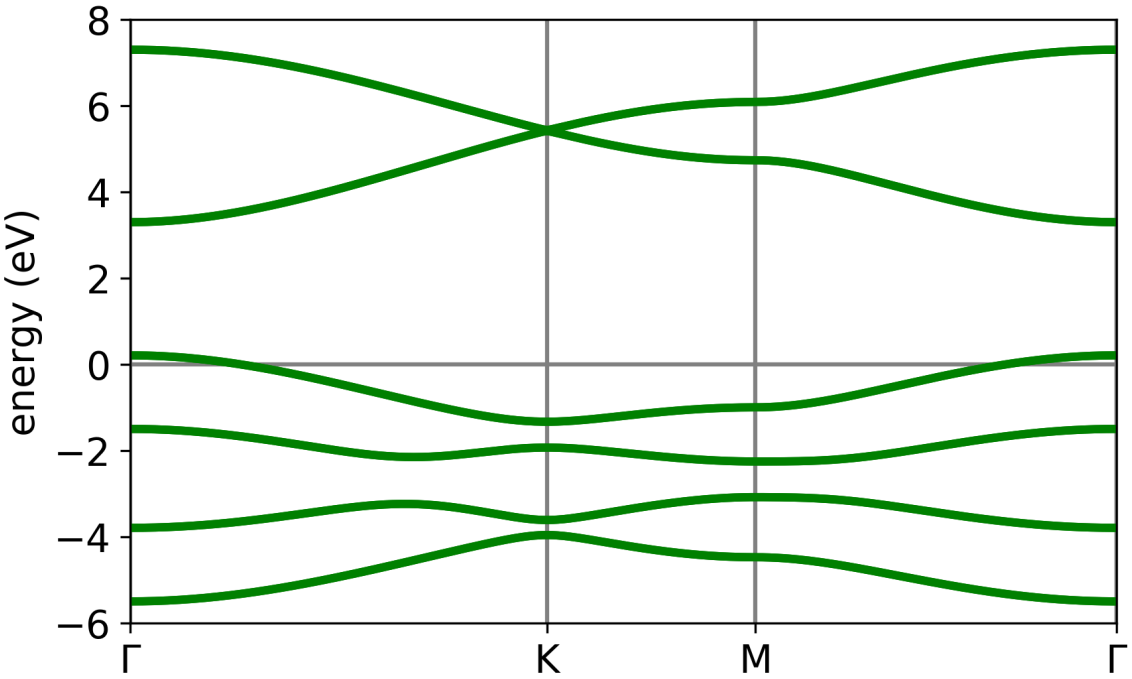

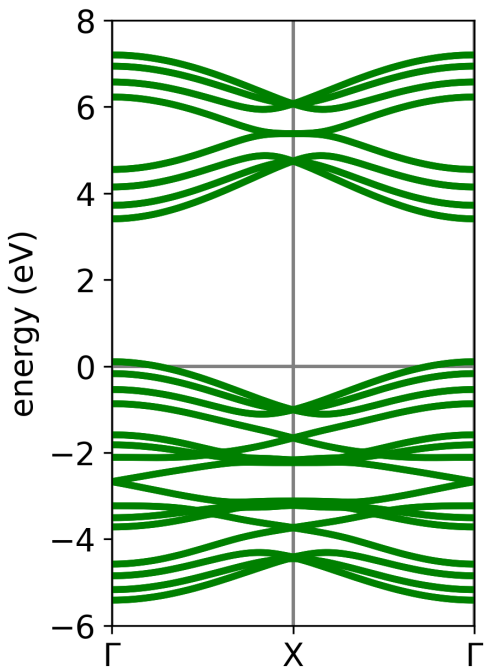

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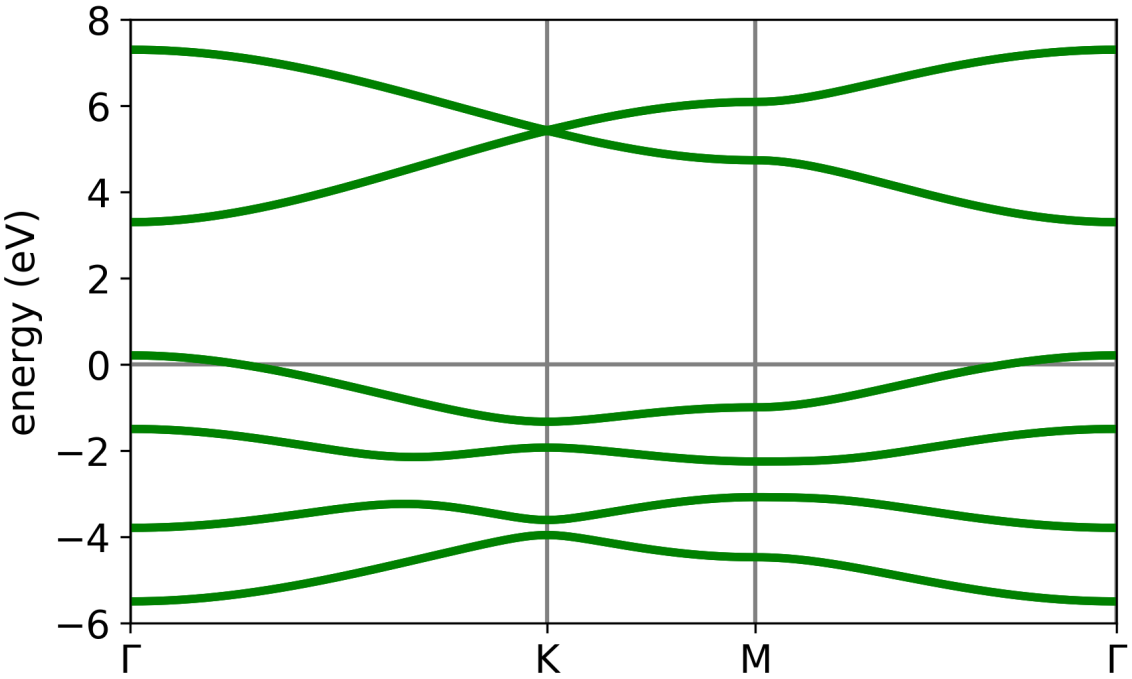

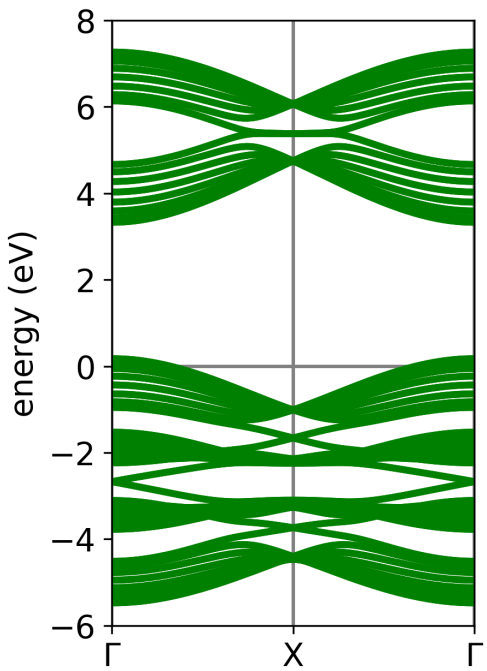

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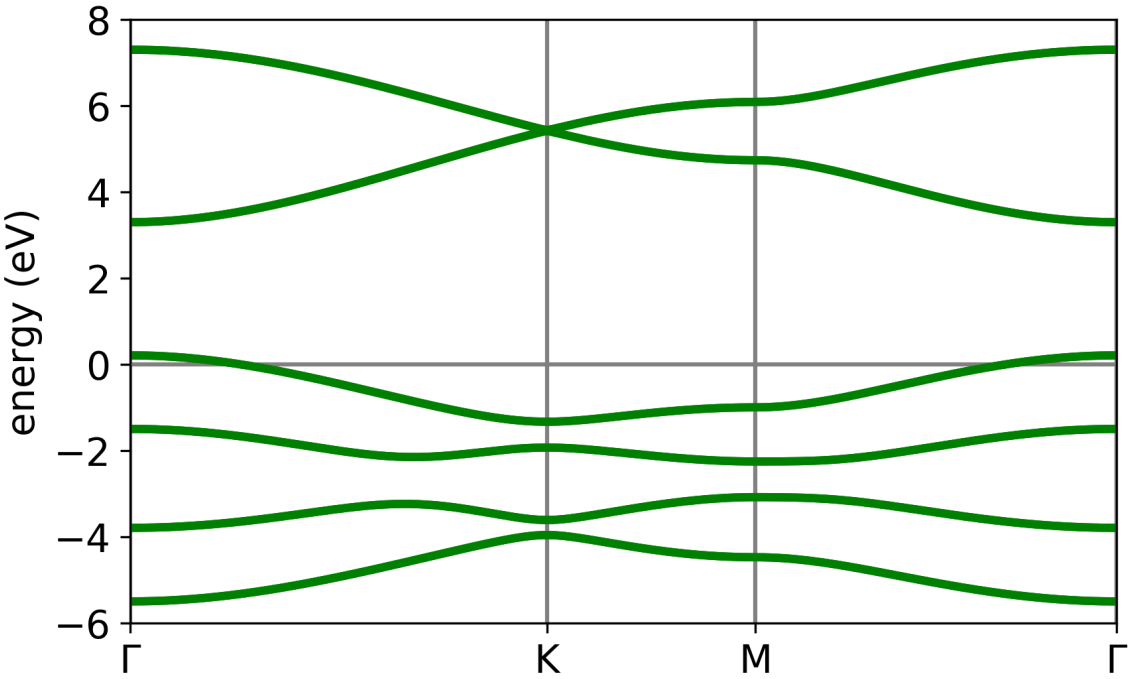

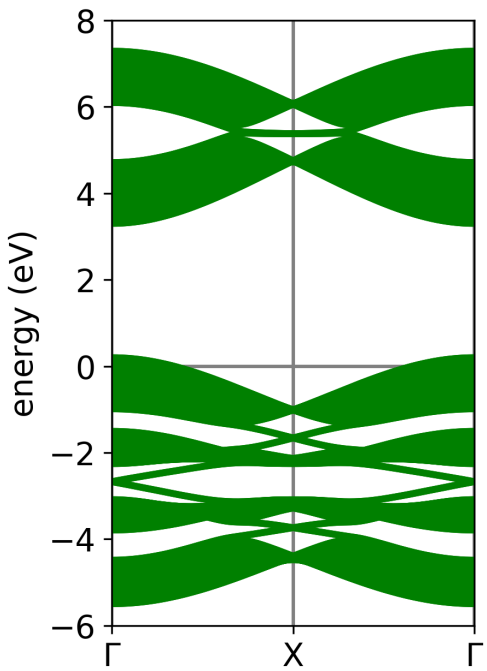

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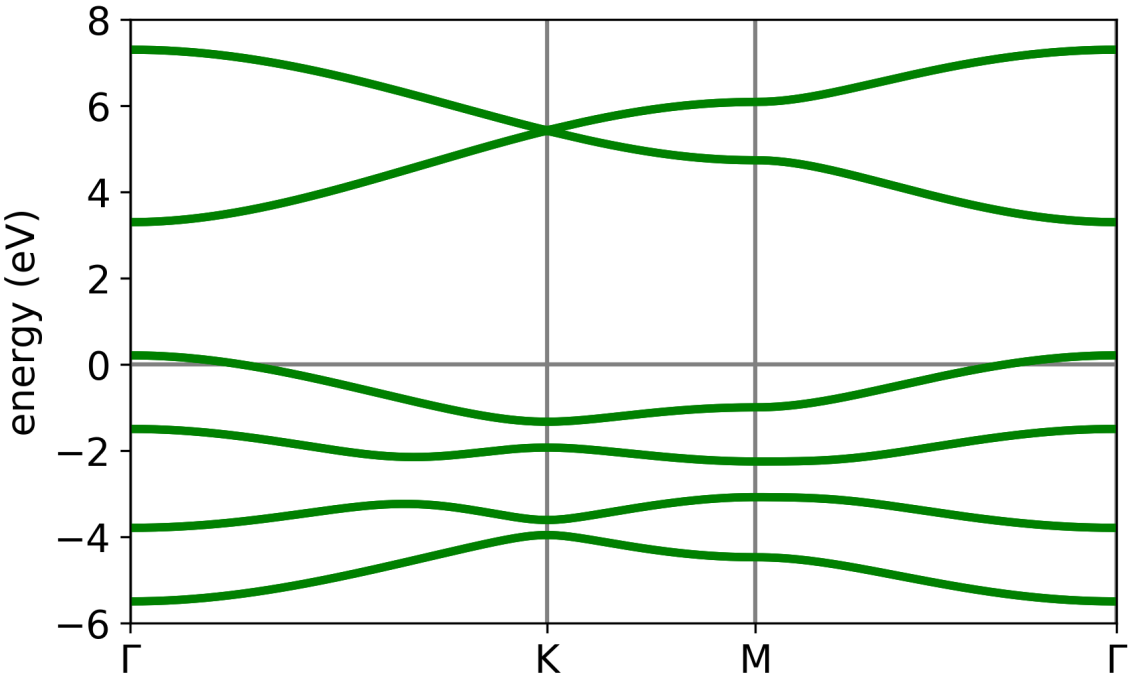

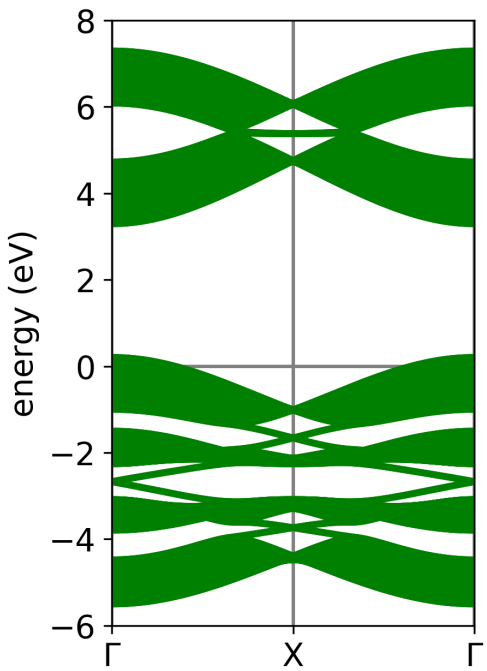

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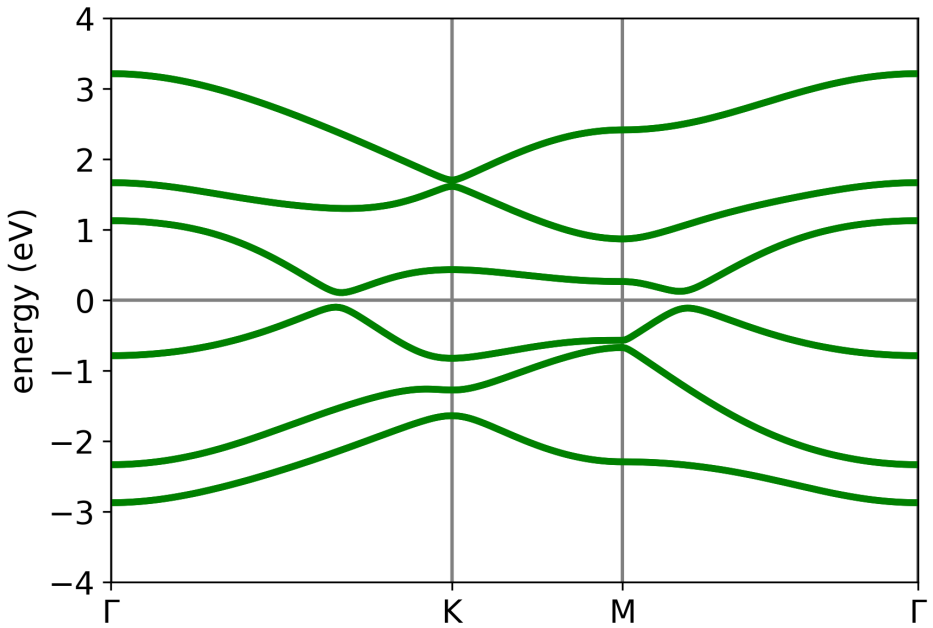

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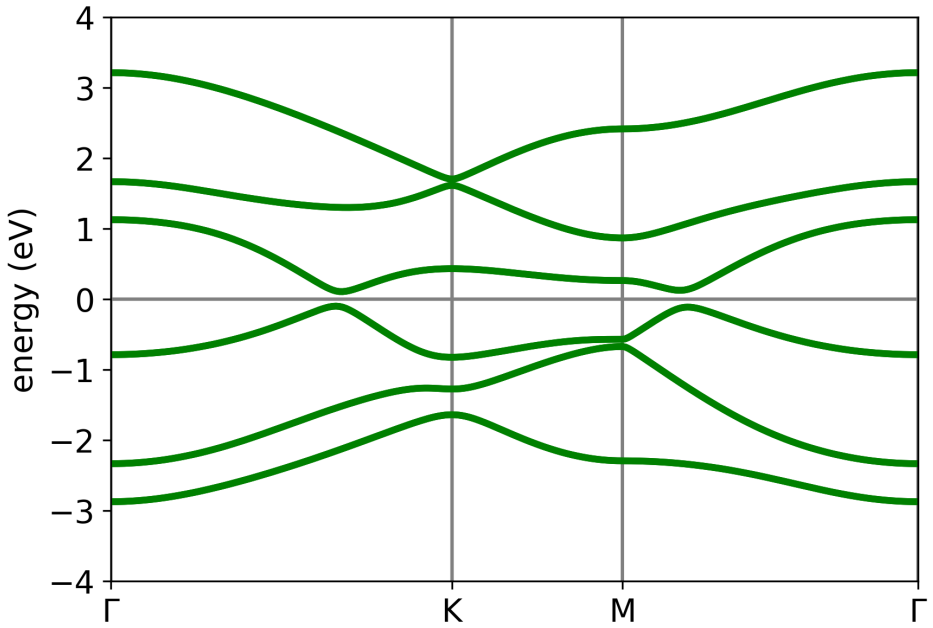

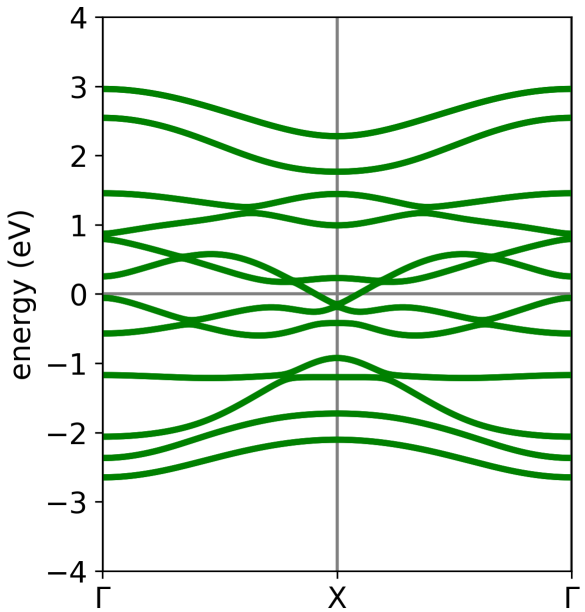

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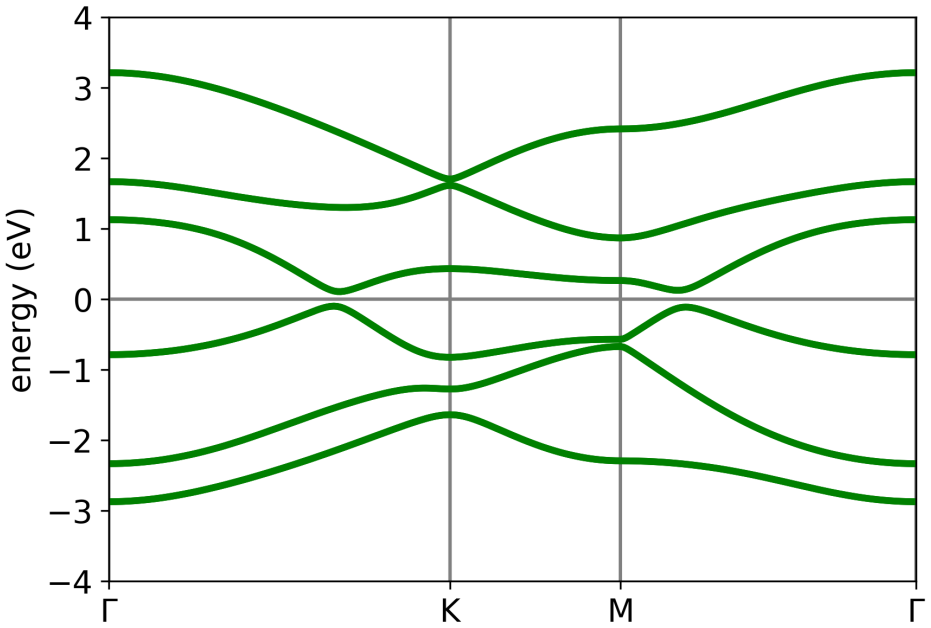

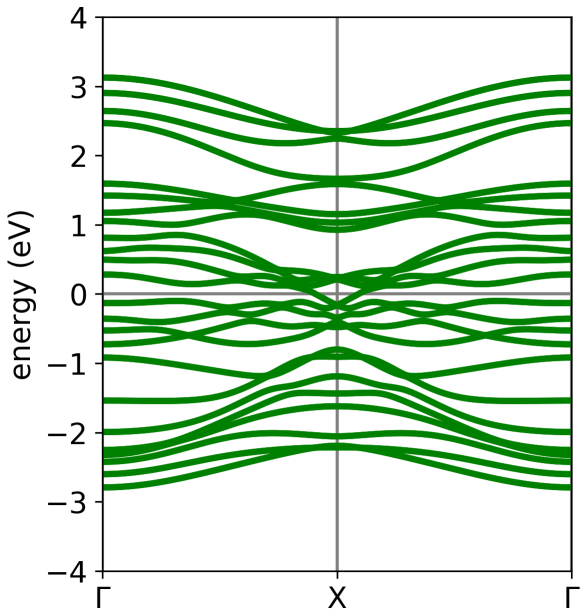

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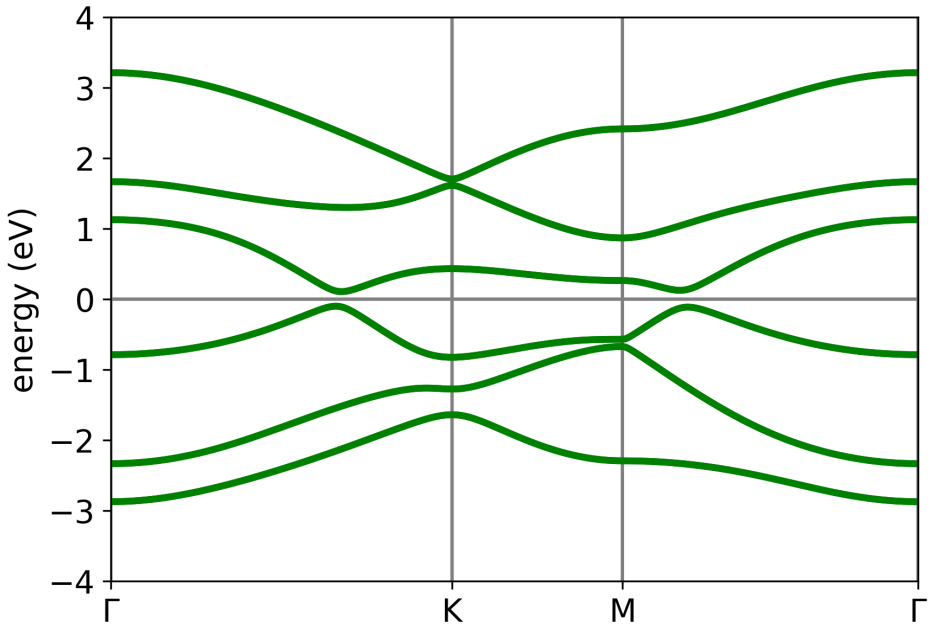

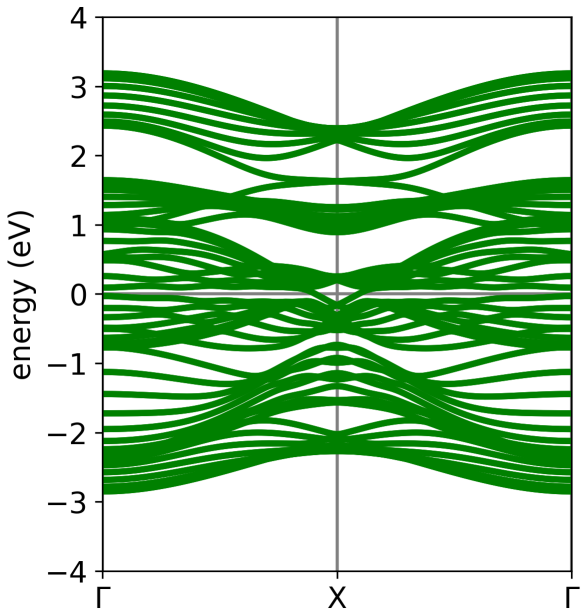

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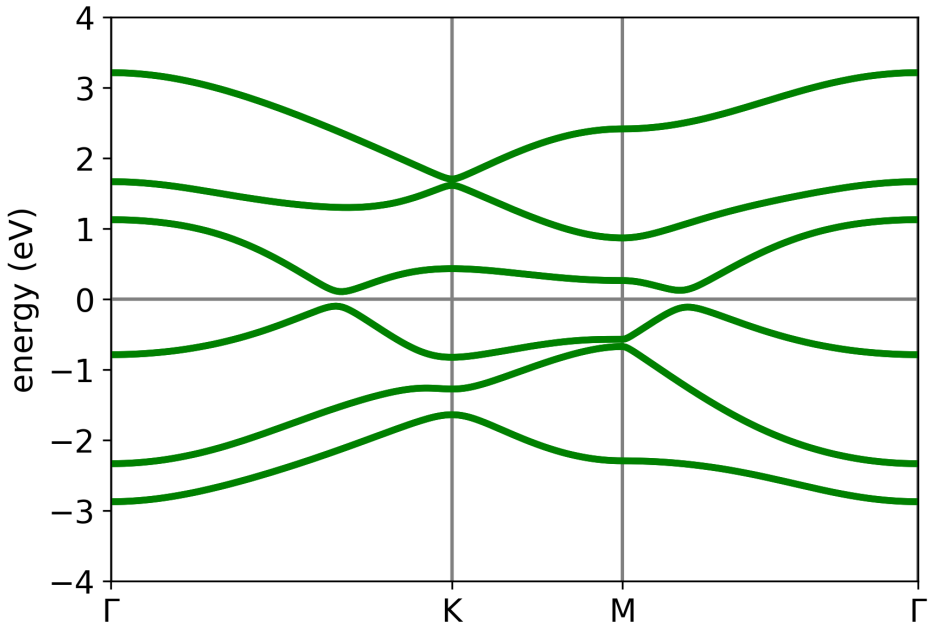

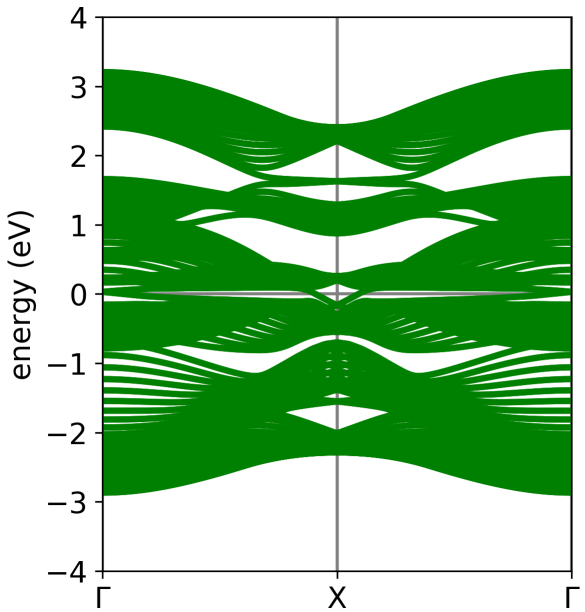

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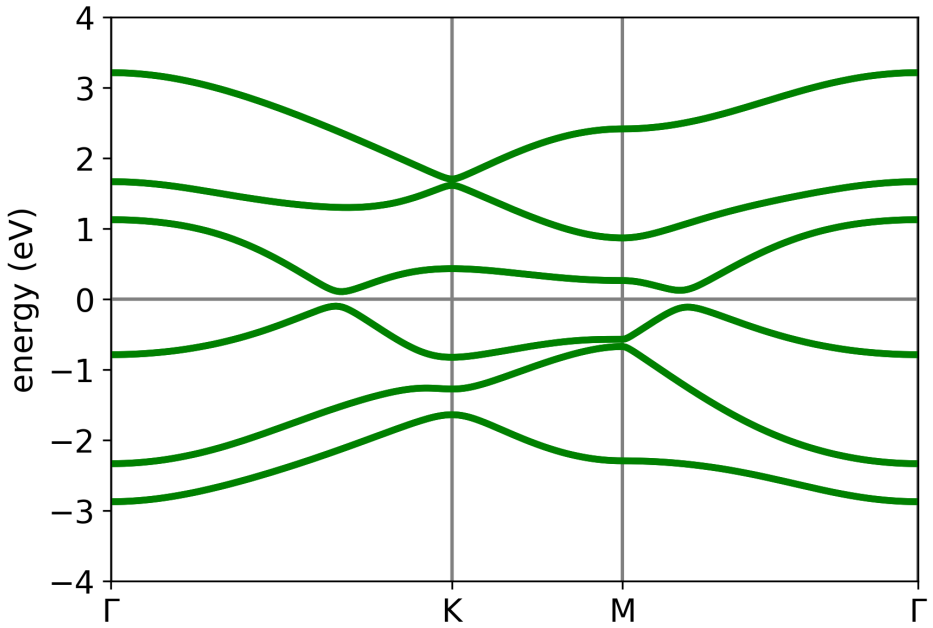

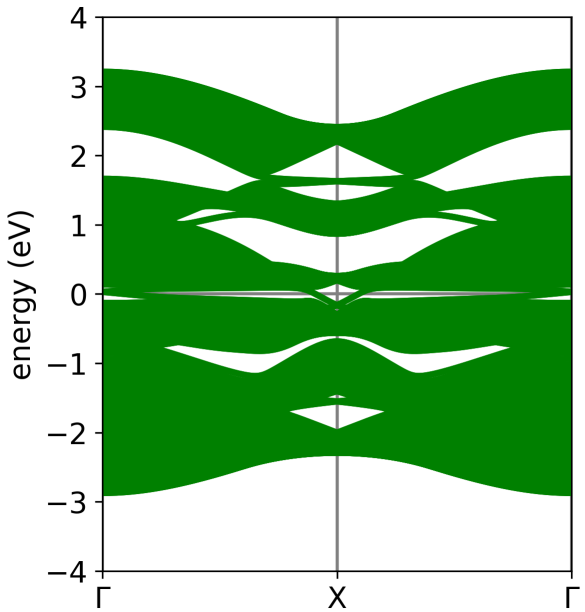

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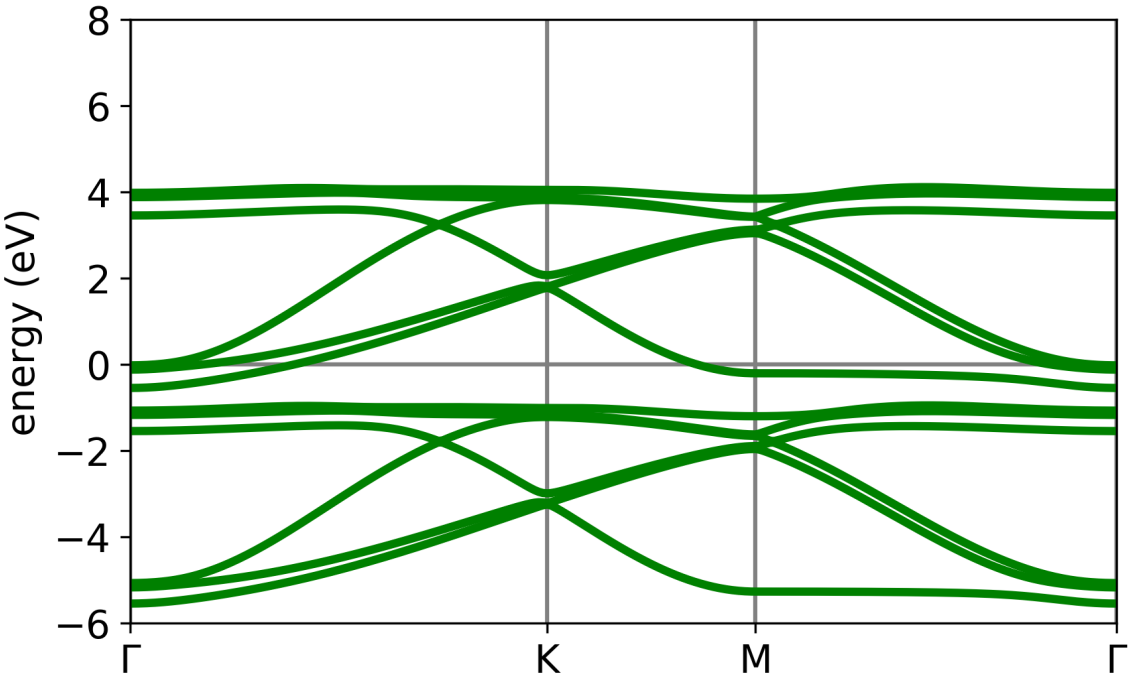

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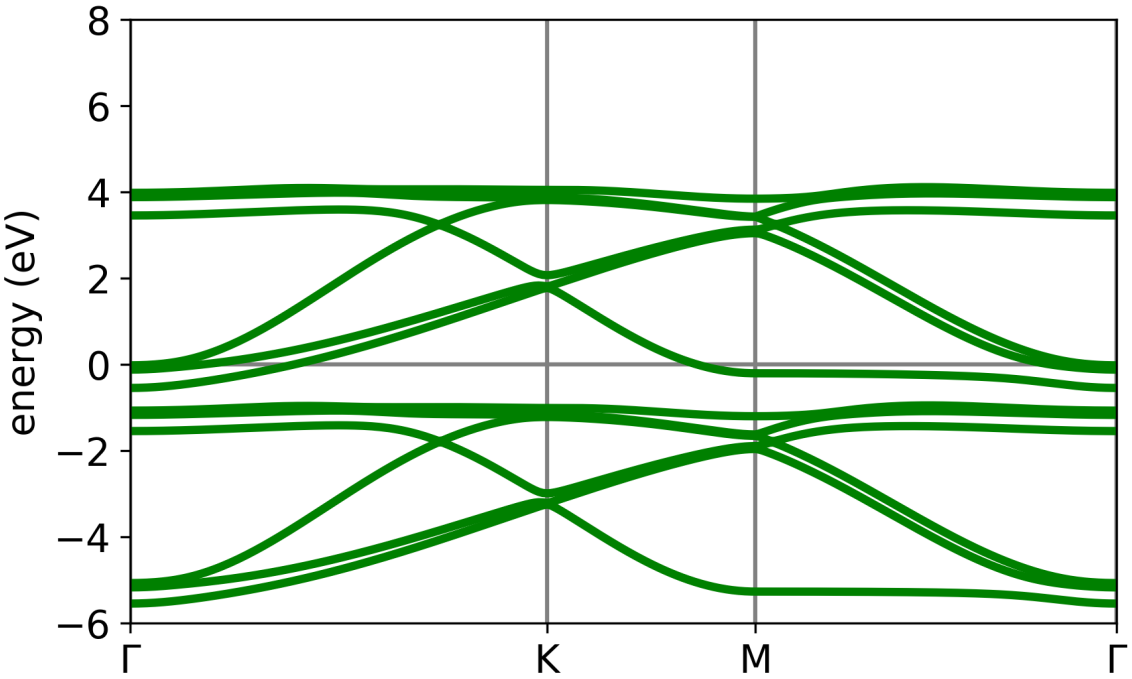

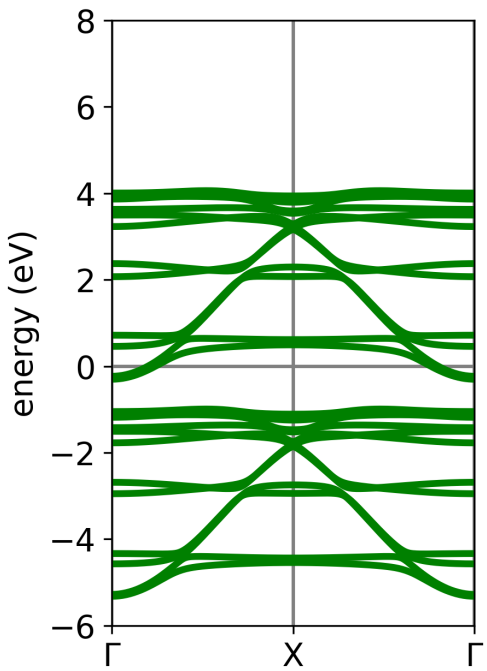

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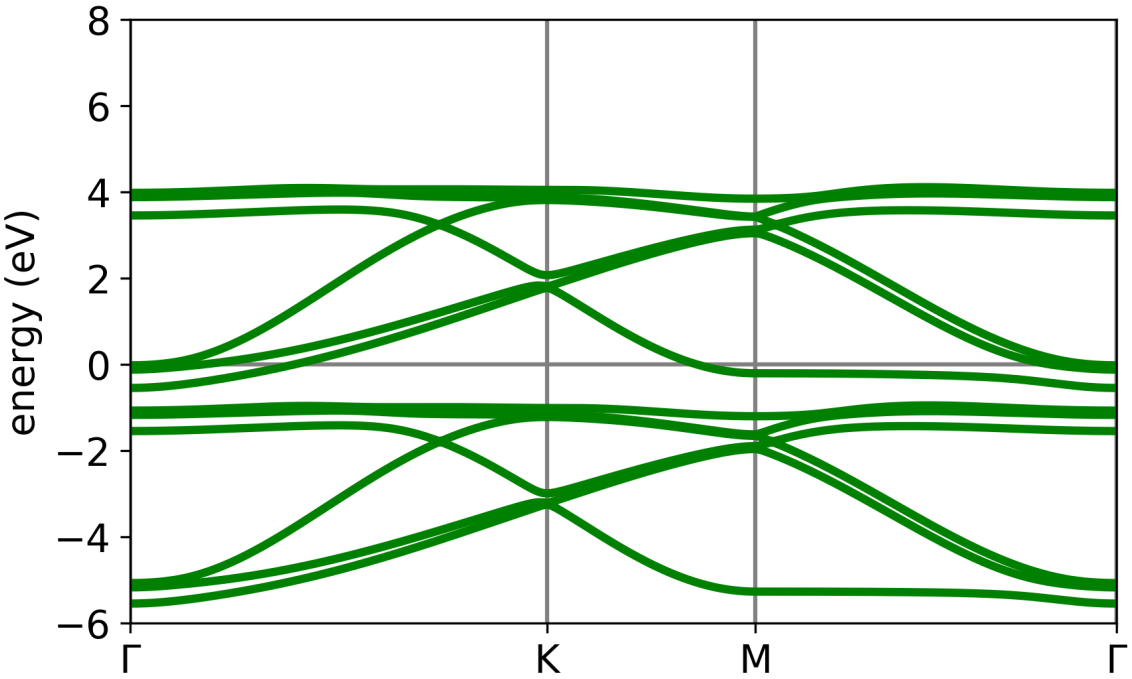

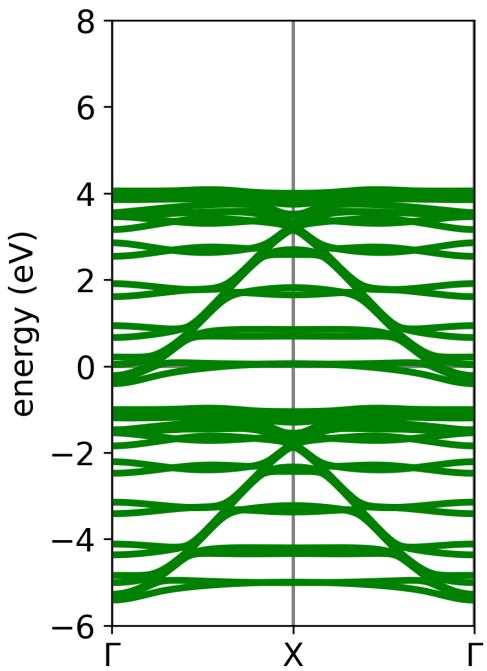

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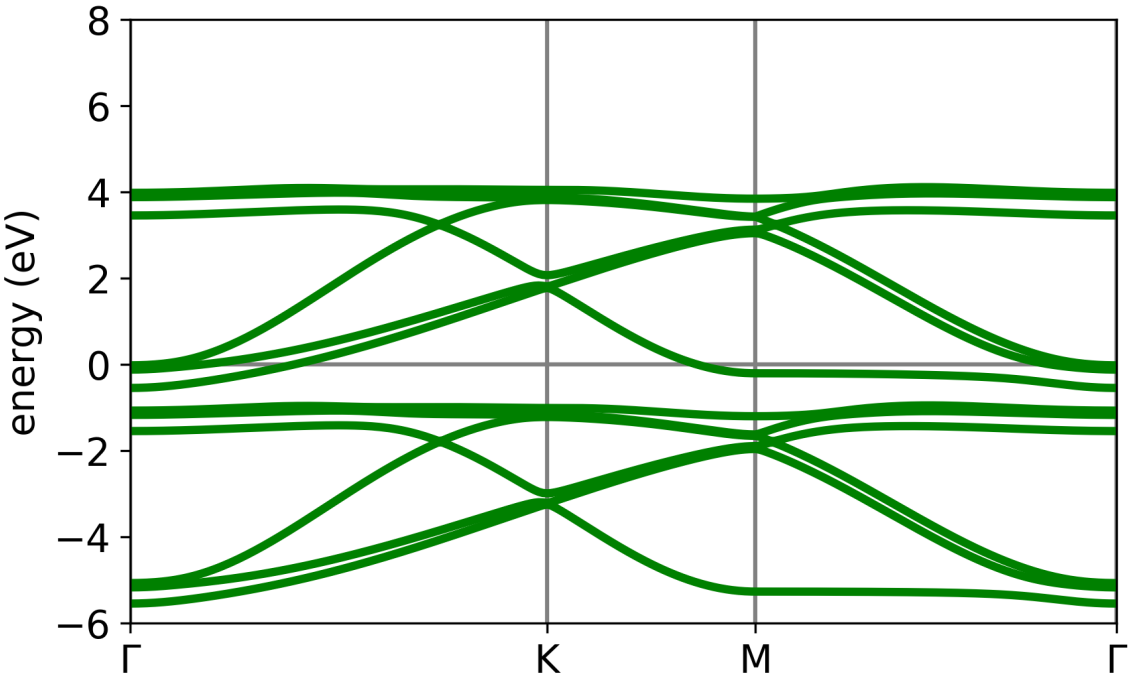

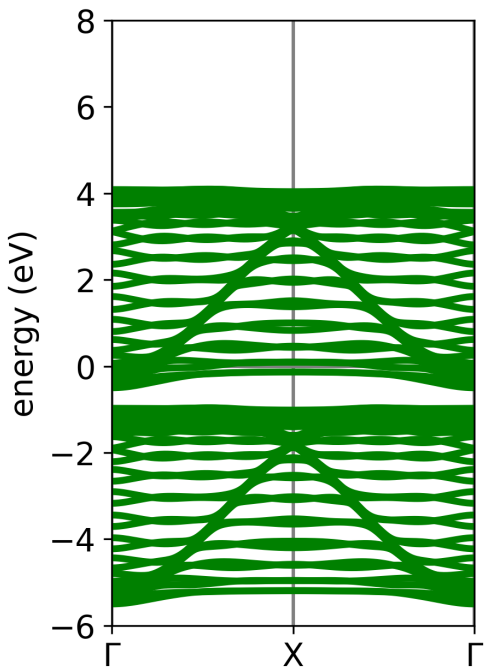

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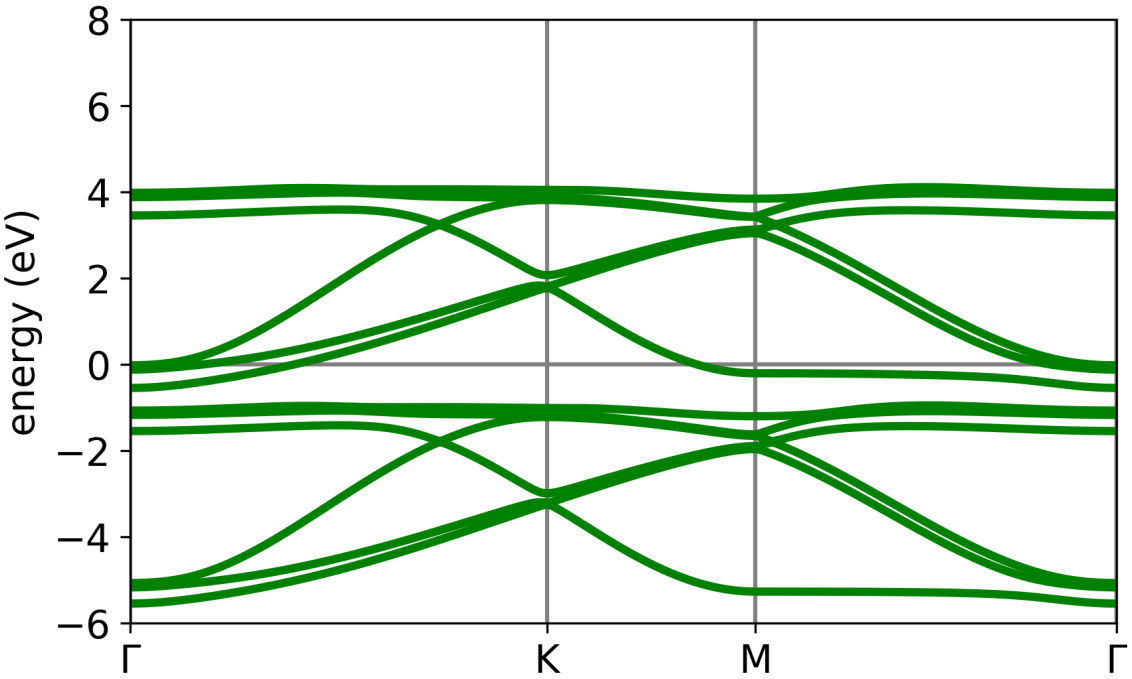

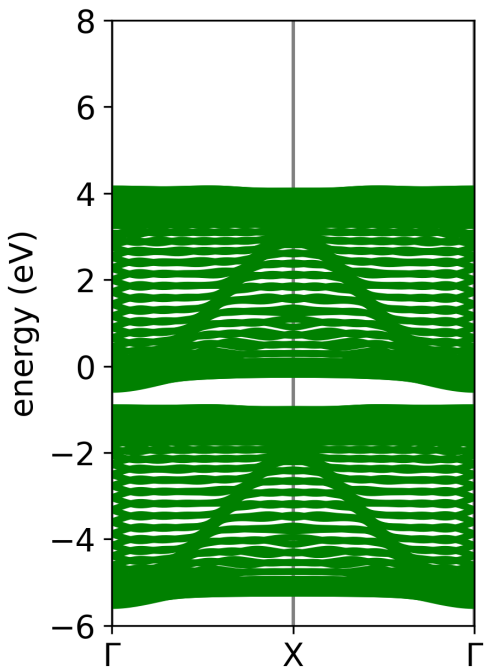

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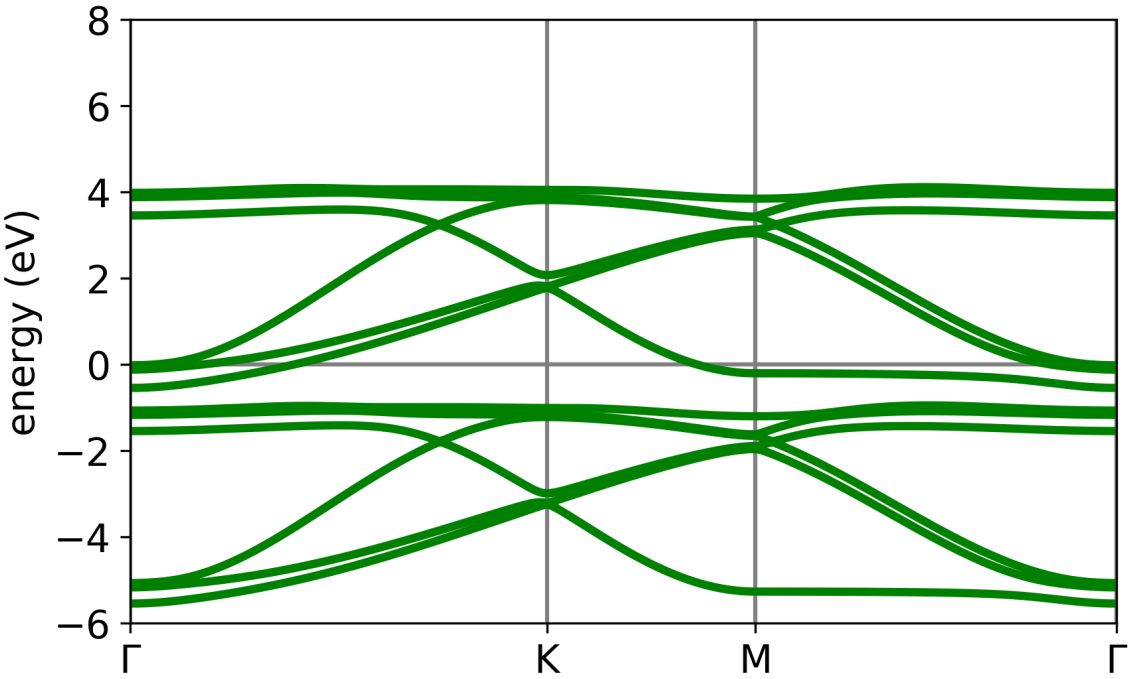
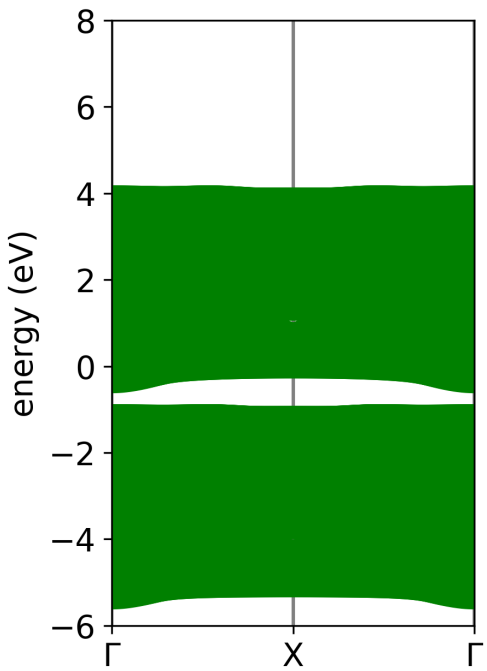
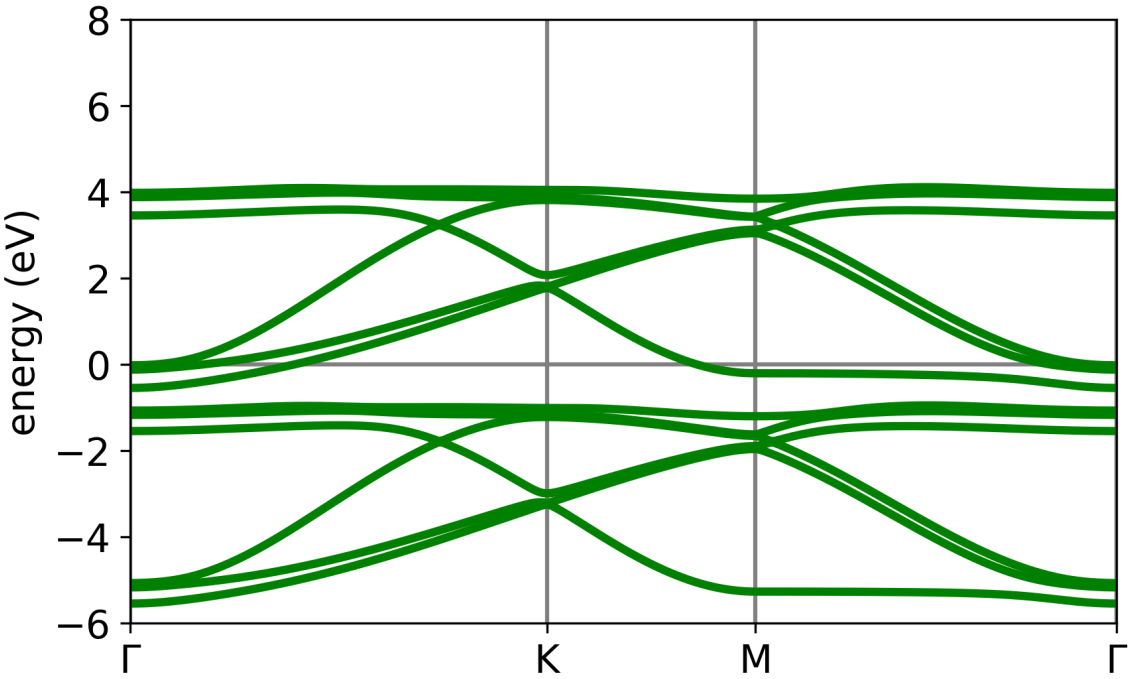
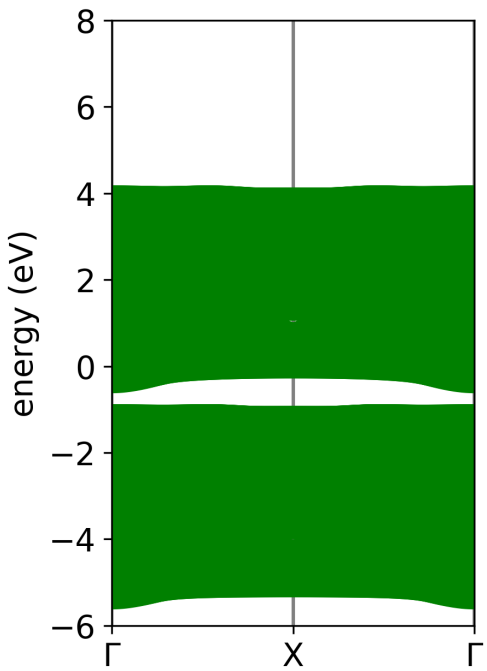




- "strong SOC" $t_1 = 1$, $\Delta_{\text{trig.}} = 1$, $\lambda = \mathbf{5}$
- "weak SOC" $t_1 = 1$, $\Delta_{\mathbf{trig.}} = \mathbf{1.5}$, $\lambda = 0.5$
- "realistic parameters" (e.g., for $SrRuO_3$ bilayers): $t_1^{\pi} = -1$, $t_2^{\sigma} = -0.5$, $\Delta_{\text{trig.}} = 0.05$, $\lambda = 0.5$, Zeeman splitting $= 5$

TB model for d electrons on a honeycomb lattice: D. Xiao *et al.*, Nat. Comm. **2**, 596 (2011)
TI (QSH) and Chern insulators (QAH) can be stabilized at different fillings





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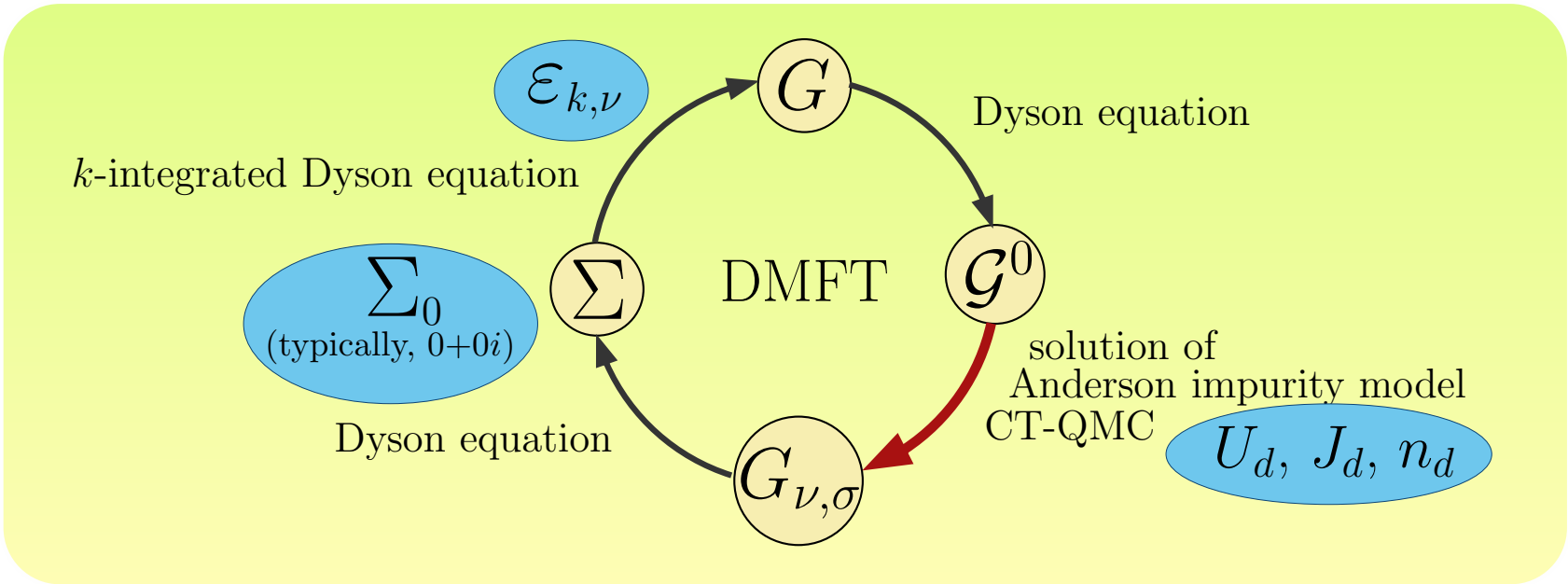
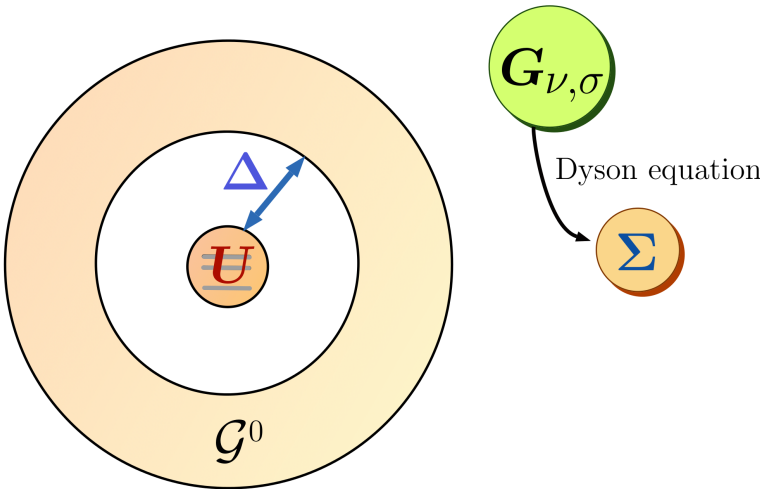
crucial:

- real structures → material-specific parameters
- realistic description of electronic correlations

Dynamical mean-field theory (DMFT)





lattice Hubbard model

↕

Anderson **impurity** model

- Mott transition
- paramagnetic state
- physics at a finite temperature

DFT+DMFT and analysis of the topology

DFT (wien2k / wien2wannier, vasp, fplo):

- DFT / DFT+U calculations
- structural relaxations in DFT+U (DFT+DMFT not feasible)
- Wannier functions $\rightarrow$ hoppings, on-site energies, SOC

DMFT (w2dynamics):

M. Wallerberger *et al.*, arXiv:1801.10209

- continuous time QMC (CT-HYB)
- Kanamori interaction
  (density-density + spin flip + pair hopping)
- t_{2g}/e_g subspace
- no charge self-consistency

topology (non-interacting):

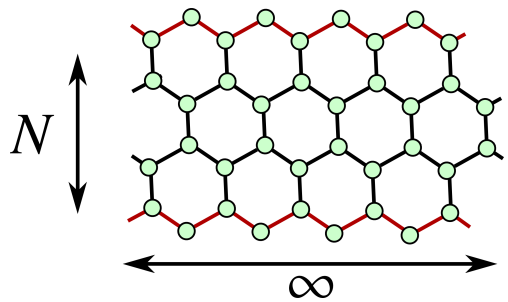
- Chern number calculations

  T. Fukui and Y. Hatsugai, JPSJ **76**, 053702 (2007)
- iterative Green's function

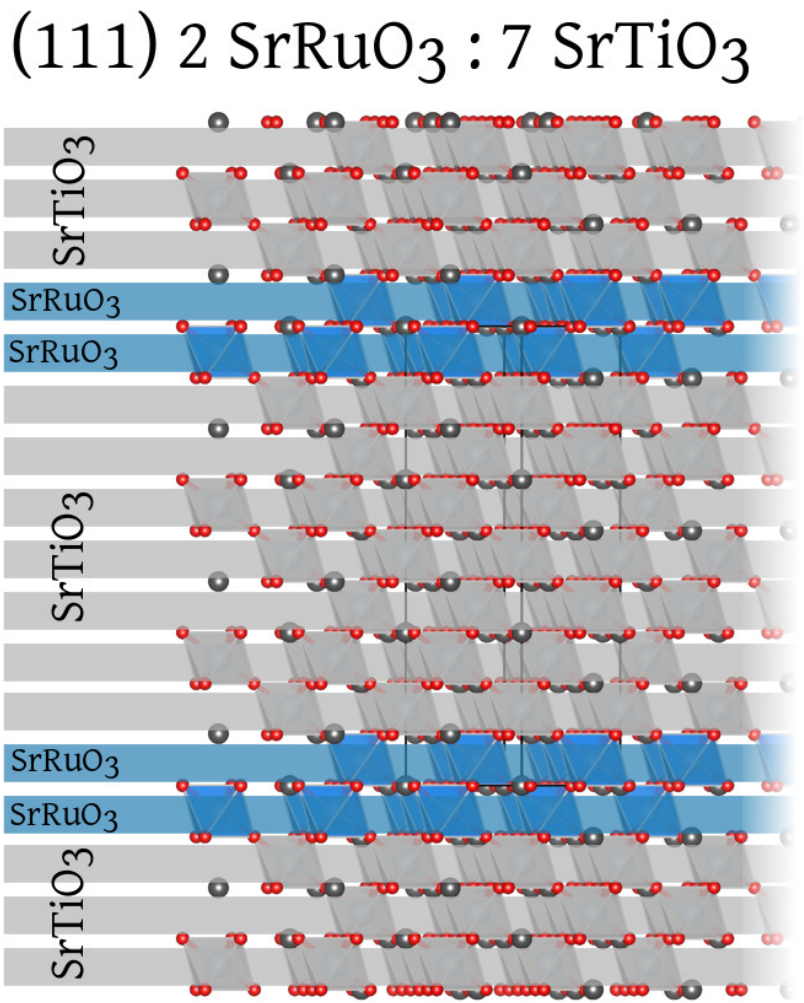
  M. L. Sancho *et al.*, J. Phys. F **15**, 851 (1985)

topology (interacting):

- direct evaluation of $A(k, \omega)$ using the DMFT self-energy on cylinders



$SrRuO_3 : SrTiO_3$



Why $SrRuO_3$?

- a correlated ferromagnetic metal ($T_C = 160\,K$) in the bulk
- t_{2g}^4 with a moderate SOC — a promising TI candidate

  D. Xiao *et al.*, Nat. Comm. **2**, 596 (2011)
- good quality heterostructures

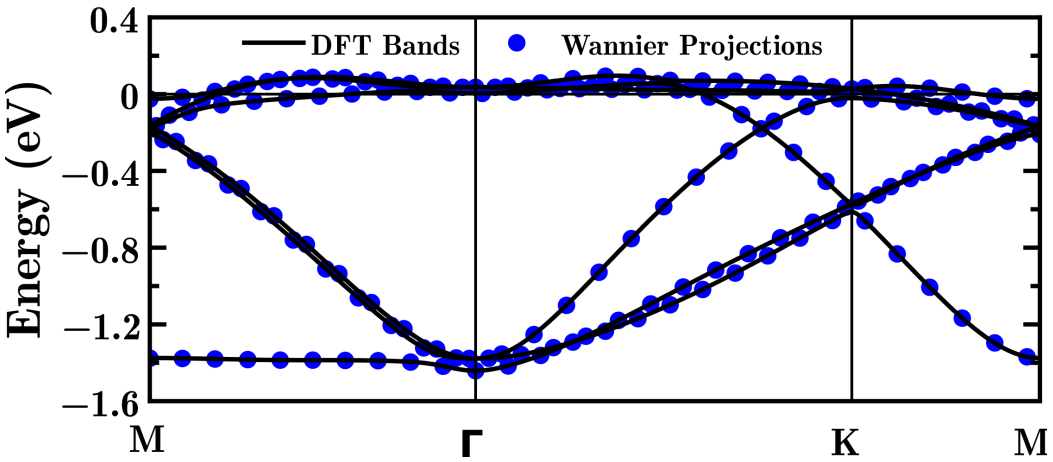
  G. Koster *et al.*, RMP **84**, 253 (2012)

Why DFT+DMFT?

- reproduces T_C in bulk $SrRuO_3$
- captures the AF insulating state of ultra-thin (001) SRO:STO

  L. Si *et al.*, PRB **92**, 041108(R) (2015)

$SrRuO_3 : SrTiO_3$: DFT+DMFT results

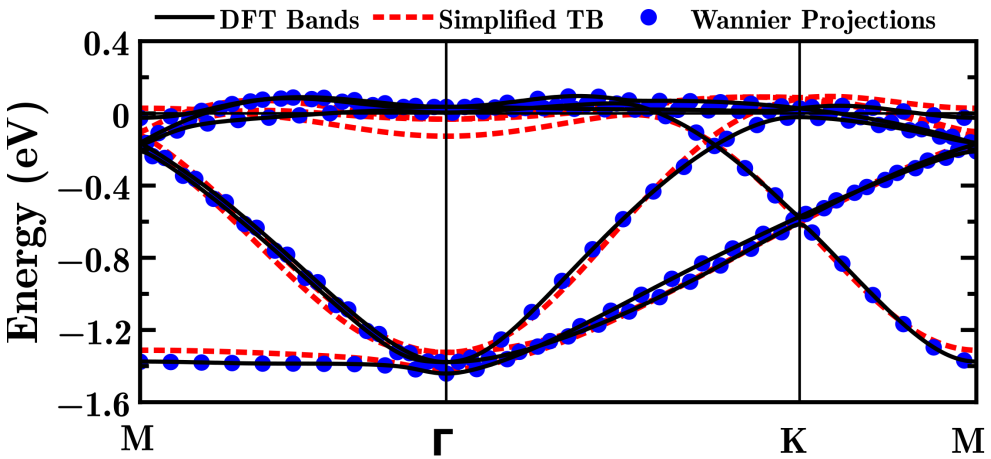


DFT

- separated 6-band manifold (2 Ru, t_{2g} only)
- a Dirac point (Γ–K)

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

$SrRuO_3 : SrTiO_3$: DFT+DMFT results



DFT

- separated 6-band manifold (2 Ru, t_{2g} only)
- a Dirac point (Γ–K)
- good description with only four parameters:

ε_0	-410 meV
t_1^σ	-225 meV
$\mathbf{t_2^\sigma}$	$\mathbf{-175}$ **meV**
$\mathbf{\Delta_{trig.}}$	**15 meV**

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

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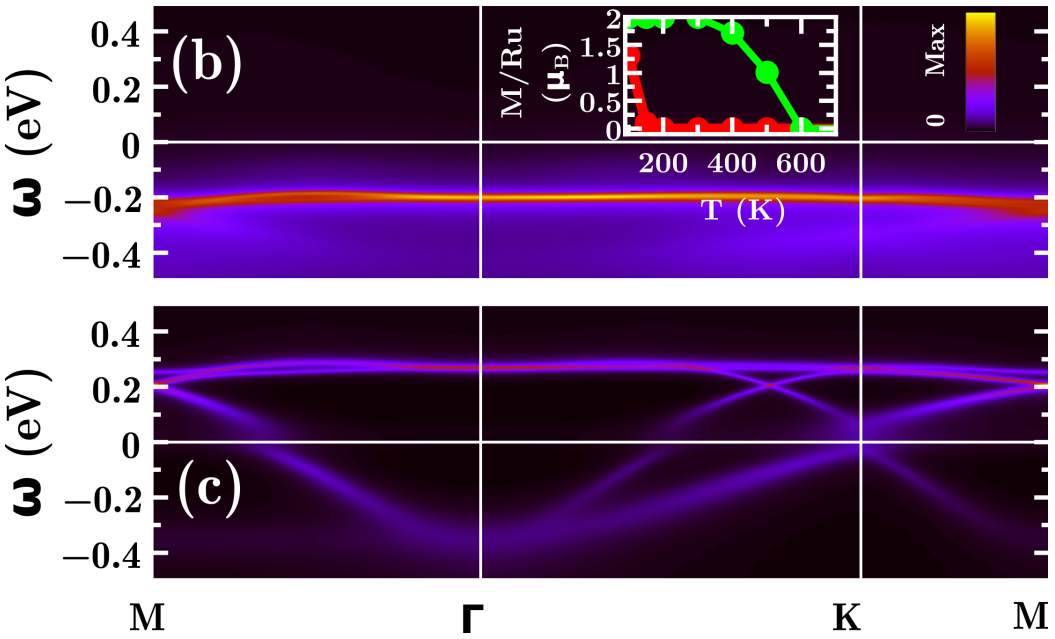

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DMFT

- half-metallic FM at RT (even better than bulk!)
- weak renormalization in the minority channel

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

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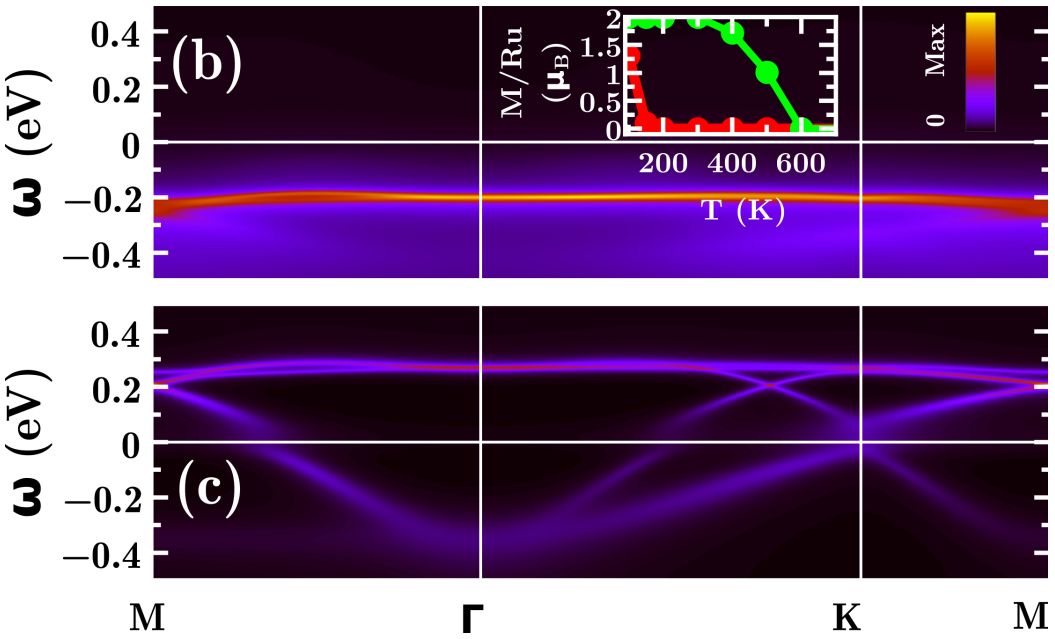

— What happens to if we include SOC?

DFT

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- a Dirac point (Γ–K)
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L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

$SrRuO_3 : SrTiO_3$: edge state calculations

- SOC opens a small gap at the Dirac point: **Chern insulator/QAH?**

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

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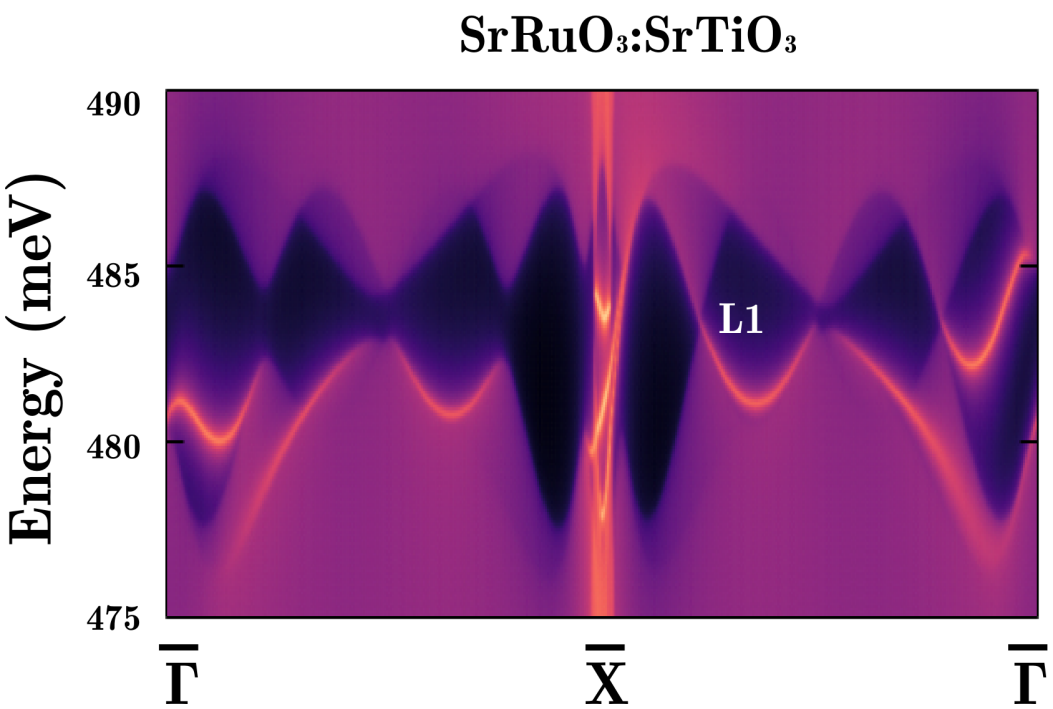

- SOC opens a small gap at the Dirac point: **Chern insulator/QAH?**
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L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

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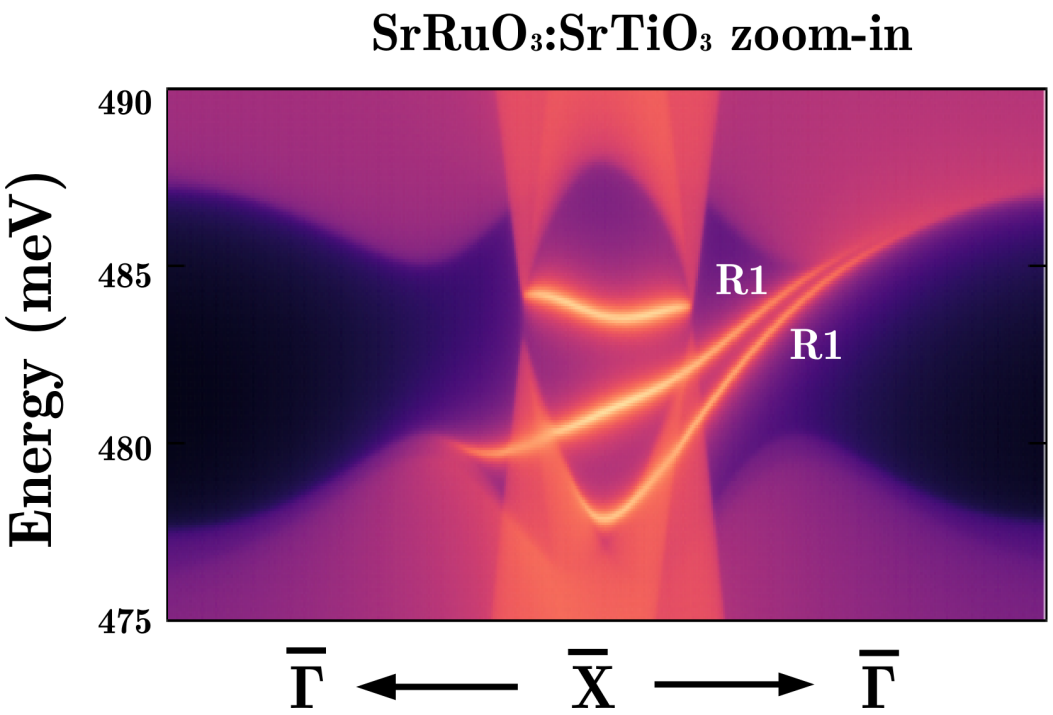

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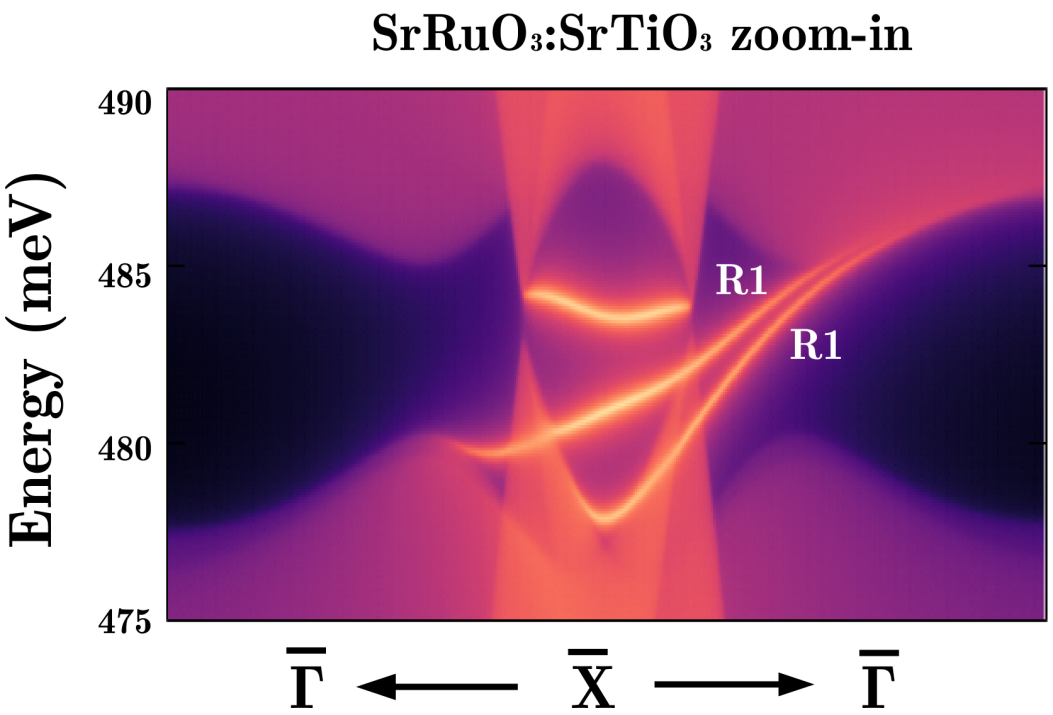

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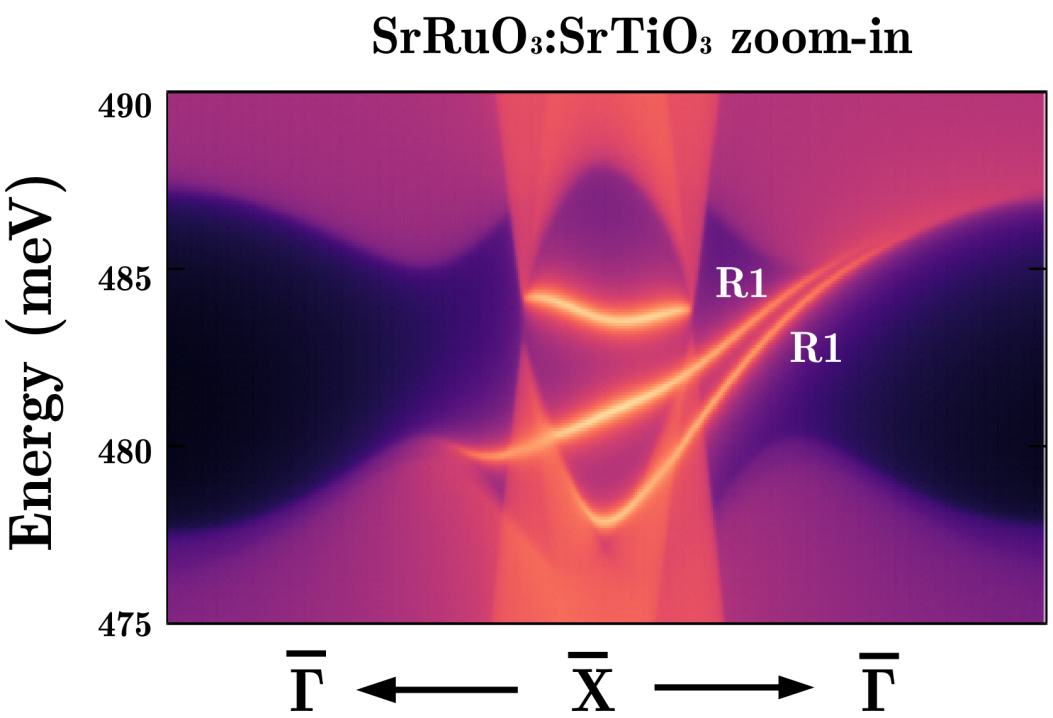

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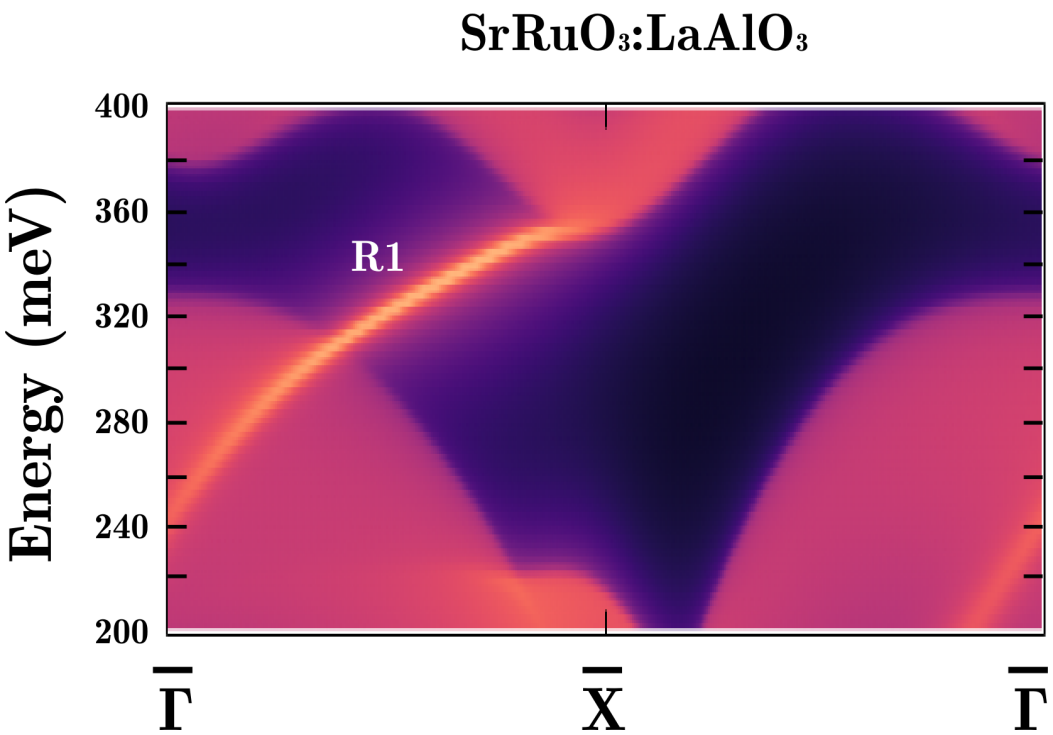
L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

$SrRuO_3 : SrTiO_3$: edge state calculations



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two promising routes:

- a different substrate ($LaAlO_3$)

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

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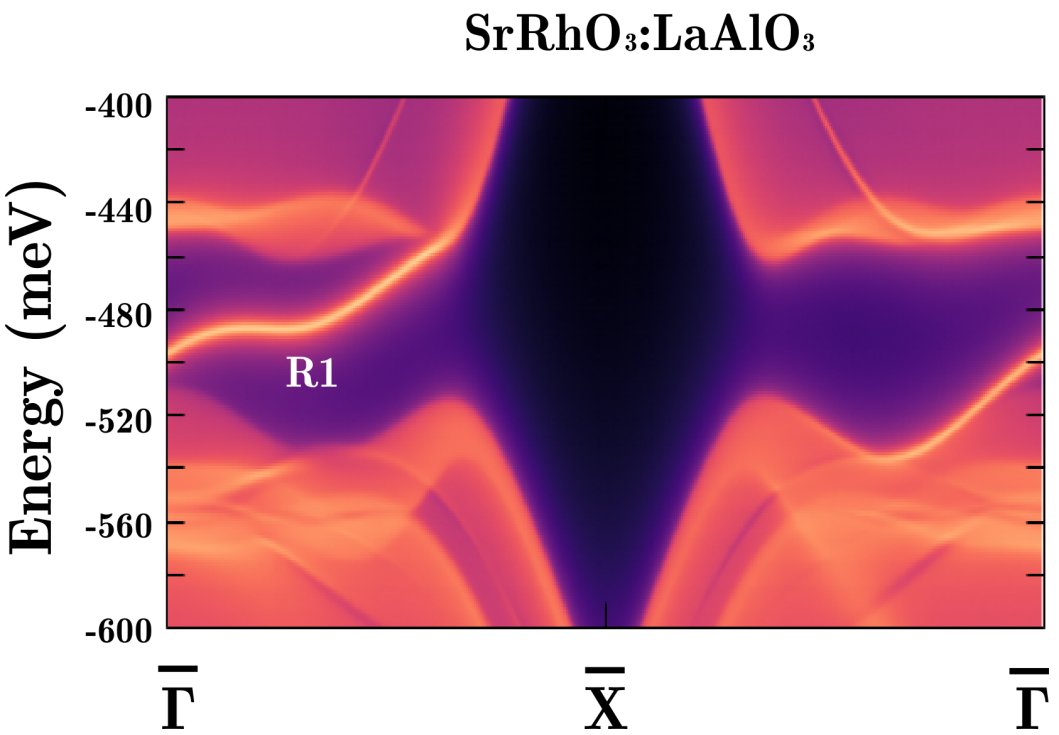

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- there are trivial and topological edge states
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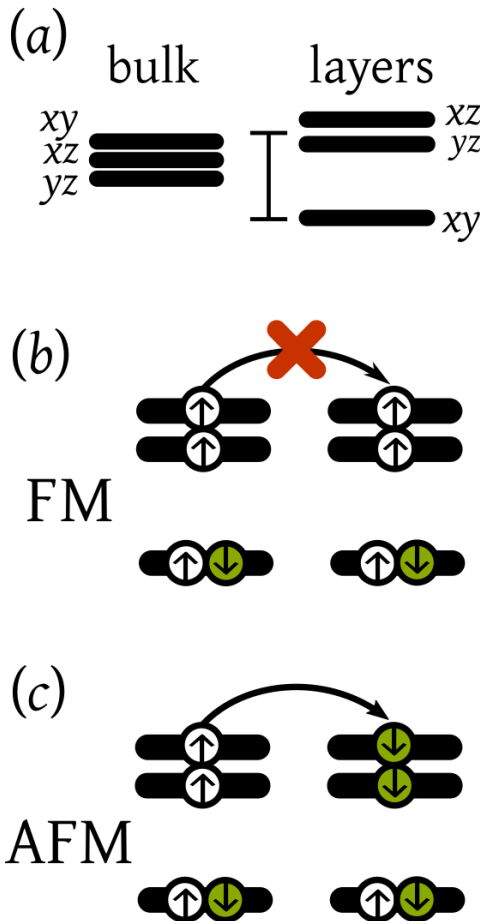
two promising routes:

- a different substrate ($LaAlO_3$)
- a different *d*-metal ($SrRhO_3$)

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

$SrRuO_3 : SrTiO_3$: summary



OJ, Z. Zhong, G. Sangiovanni, and K. Held, Dynamical mean field theory for oxide heterostructures (Springer Ser. Mater. Sci. **266**, 2018, pp. 215–243)

Ferromagnetism:

- bulk $SrRuO_3$ — t_{2g} nearly degenerate
- (001) heterostructures (AF insulators): dimensional reduction + CF splitting $\rightarrow$ orbital degeneracy is lifted
- (111) heterostructures: orbital degeneracy is protected $\rightarrow$ stable ferromagnetism

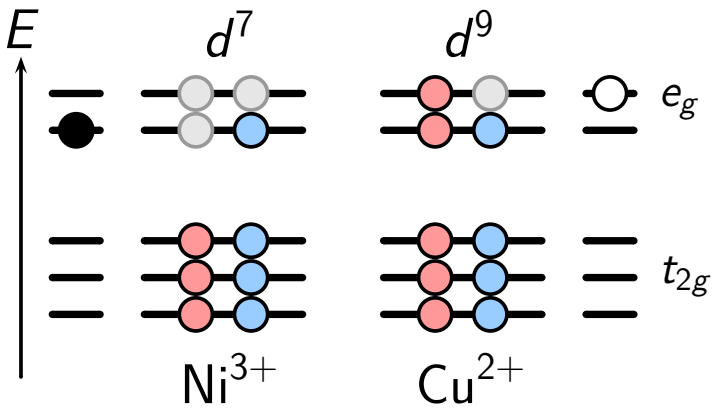
Topology:

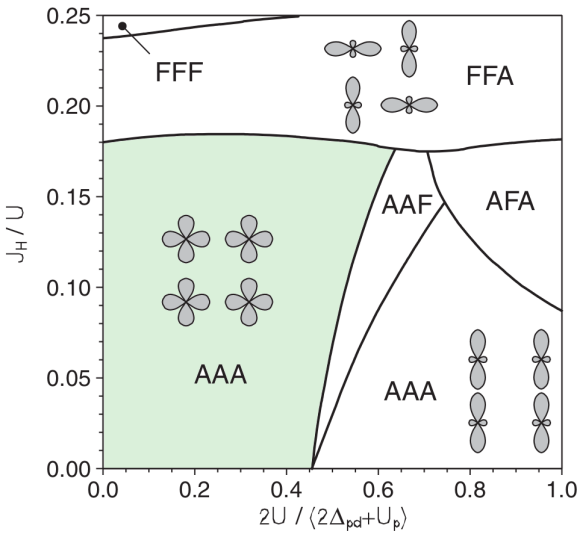
- the gap depends on both SOC and $\Delta_{\text{trig.}}$
- topology is sensitive to the sign of $\Delta_{\text{trig.}}$ and to long-range hoppings beyond the t_1–t_2 model
- further microscopic analysis is necessary

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

Why nickelates?

conjecture on cuprate-like Fermi surfaces in artificially designed nickelate superlattices



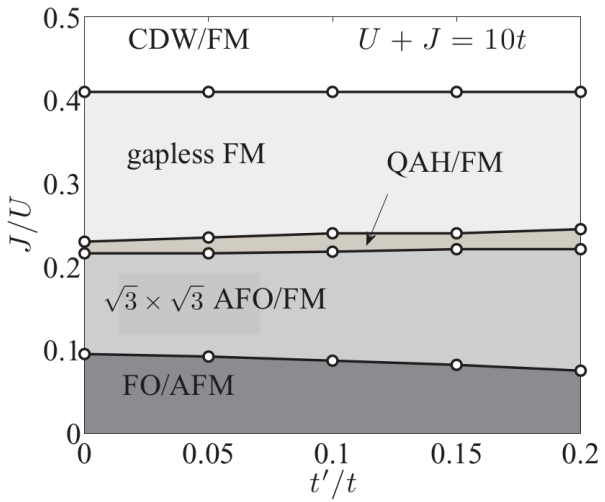


J. Chaloupka and G. Khaliulin, PRL **100**, 016404 (2008)

(001) heterostructures: d vs. $d+p$

P. Hansmann *et al.*, PRL **103**, 016401 (2009), PRB **82**, 235123 (2010); M. J. Han *et al.*, PRL **107**, 206804 (2011); N. Parragh *et al.*, PRB **88** 195116 (2013); A. Subedi *et al.*,PRB **91**, 075128 (2015)

(111) heterostructures:

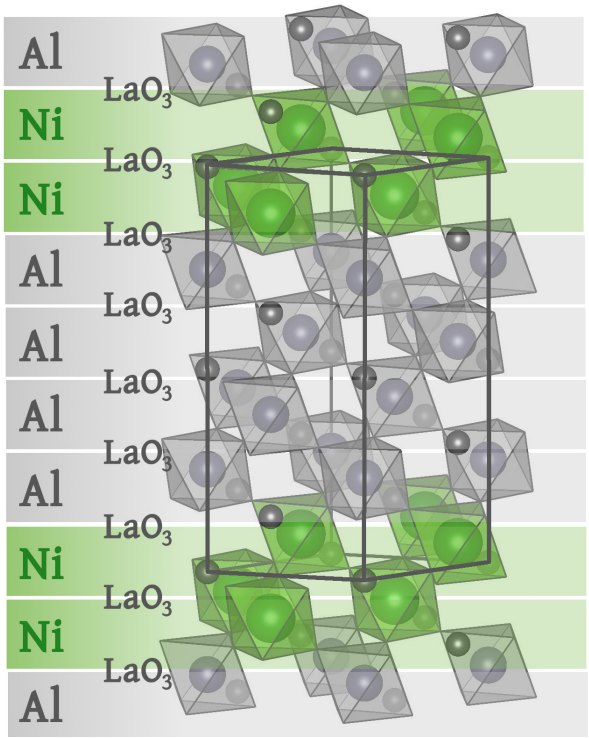


A. Rüegg *et al.*, PRB **85**, 245131 (2012)

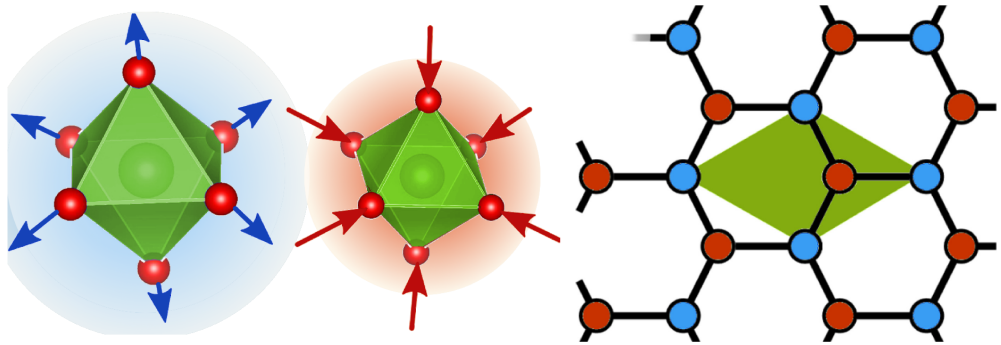
DFT+U: Dirac semimetal or a multiferroic

D. Doennig *et al.*, PRB **89**, 121110 (2014)

$LaNiO_3 : LaAlO_3$



Breathing distortion (BD)

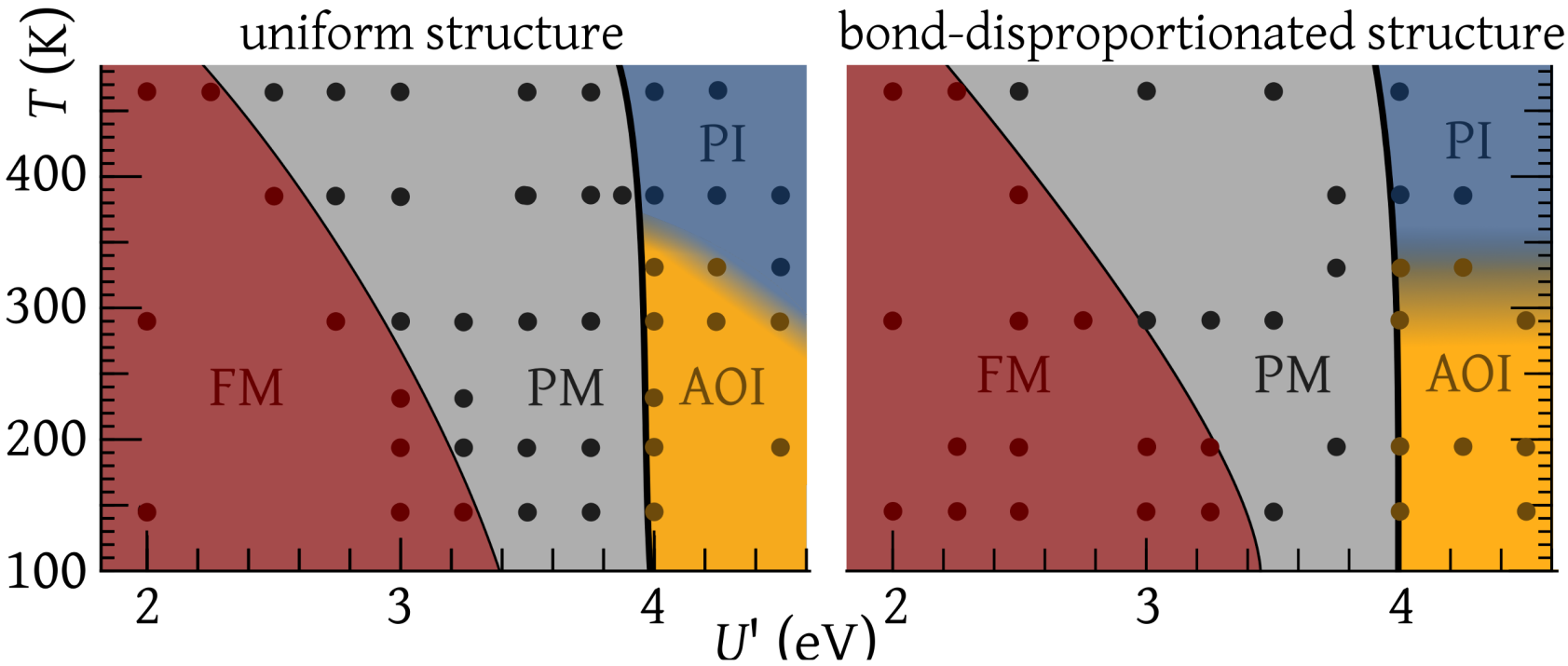


- no BD in bulk $LaNiO_3$
- strain induced by $LaAlO_3$
  $\rightarrow$ **BD is a possible scenario**
- uniform and BD are degenerate in DFT+U
  $\rightarrow$ **we study both with DMFT**

— What is the right model for nickelates?

importance of ligand holes: T. Mizokawa *et al.*, PRB **61**, 11263 (2000)
d-only model I. I. Mazin *et al.*, PRL **98** 176406 (2007)
DMFT A. Subedi *et al.*, PRB **91**, 075128 (2015)
$\rightarrow$ *d*-only model with a strongly renormalized U (**parameter in DMFT**)

$LaNiO_3 : LaAlO_3$: DMFT phase diagrams



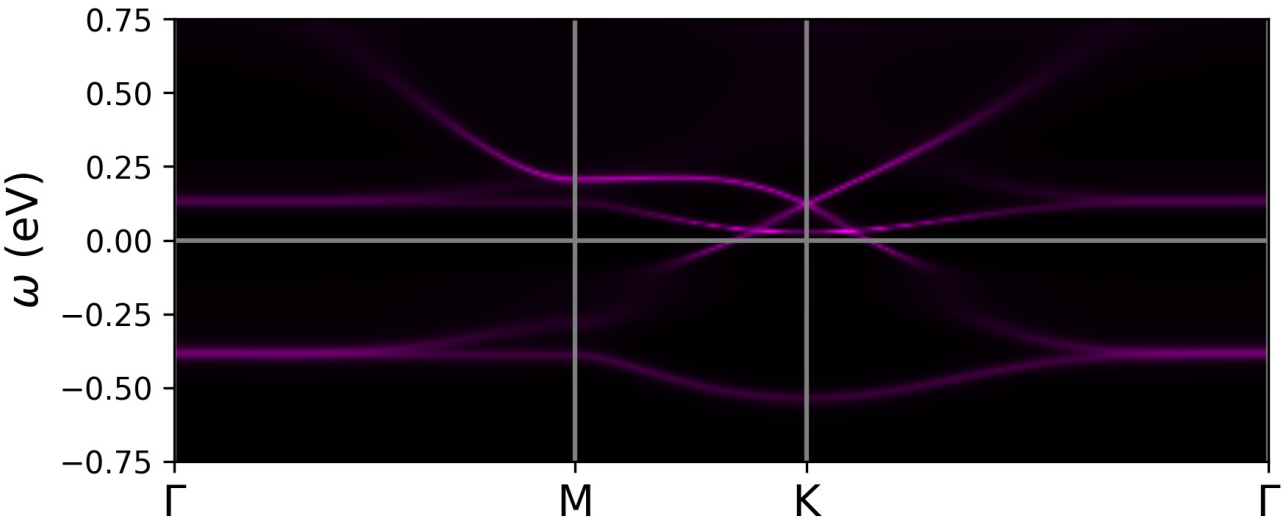
- phase diagrams are surprisingly similar
- MIT weakly depends on temperature
- four phases: a ferromagnetic (FM) and a paramagnetic metal (PM), a paramagnetic (PI) and an antiferro-orbitally-ordered insulator (AOI)

experimentally: semiconducting to insulating

S. Middey *et al.*, APL **101**, 261602 (2012); H. Wei *et al.*, APL **109**, 082108 (2016)

OJ and Karsten Held, PRB **98**, 115118 (2018)

Ferromagnetic metallic (FM) phase



- Dirac point is not at the Fermi level

OJ and Karsten Held, PRB **98**, 115118 (2018)

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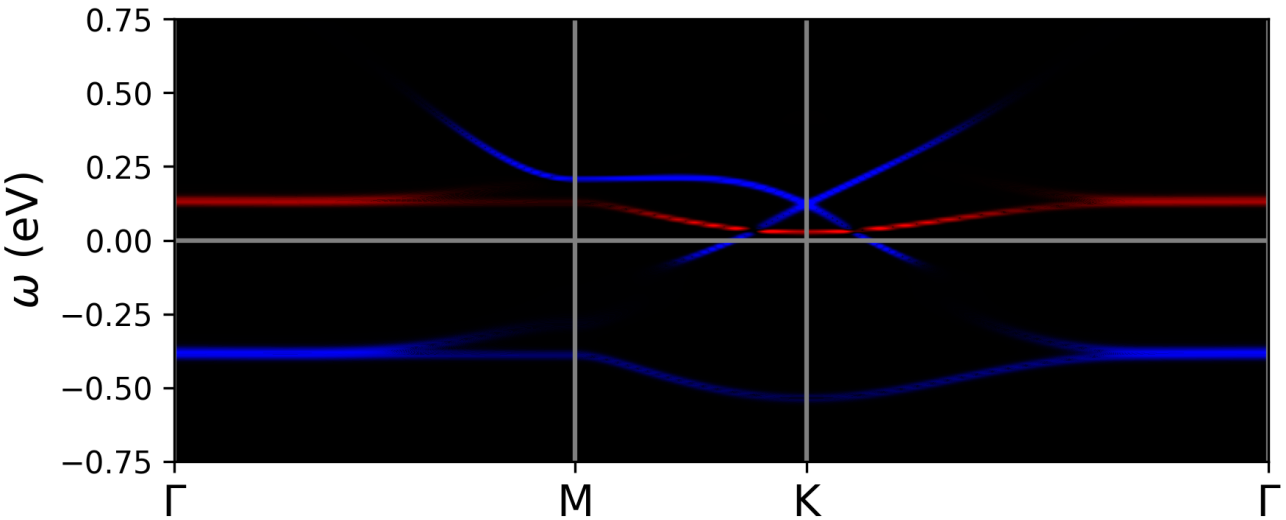

- Dirac point is not at the Fermi level
- large exchange splitting, sharp features

OJ and Karsten Held, PRB **98**, 115118 (2018)

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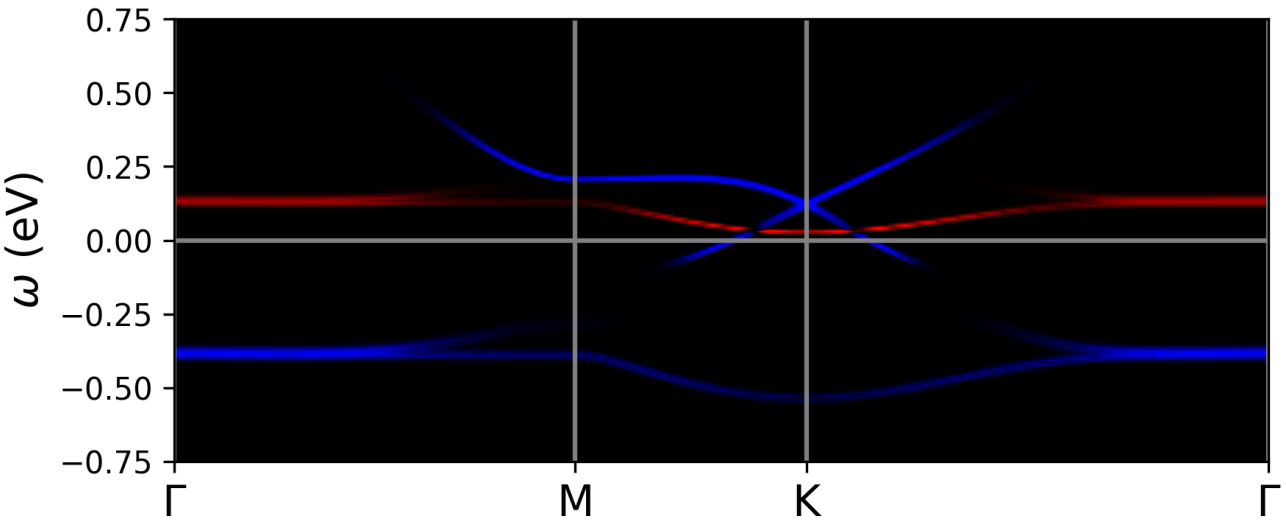

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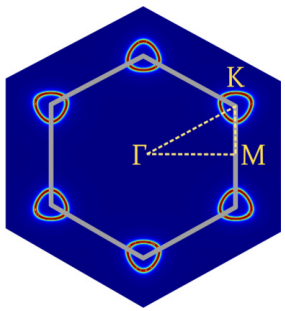

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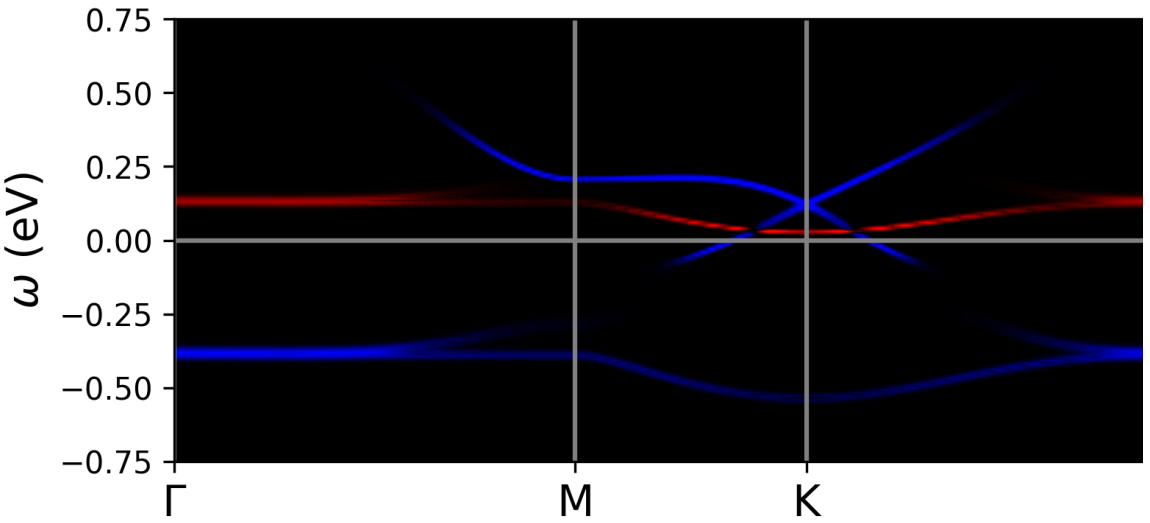

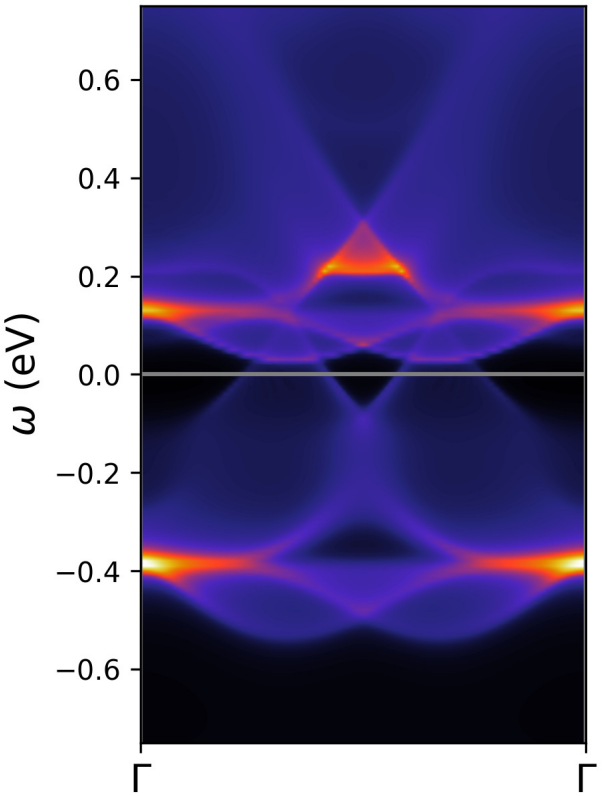

- Dirac point is not at the Fermi level
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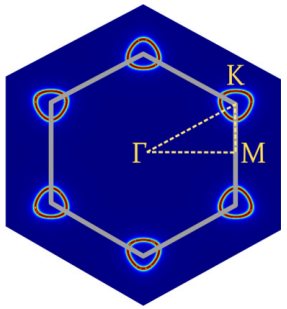
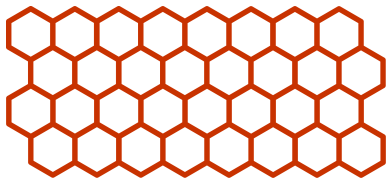
- Fermi surface differs from that of the non-interacting model
- edge states are visible in the unoccupied part of the spectrum





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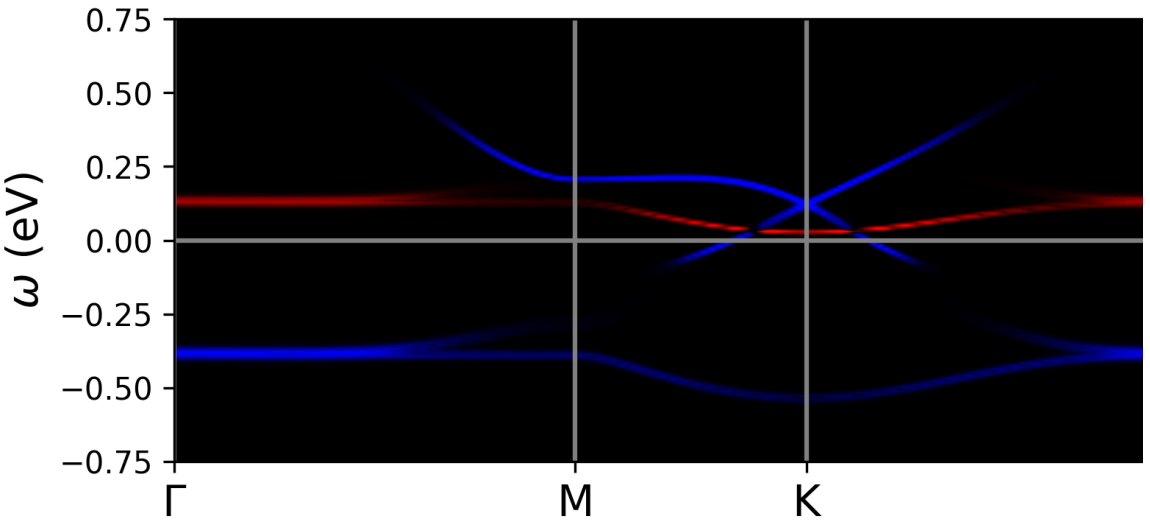

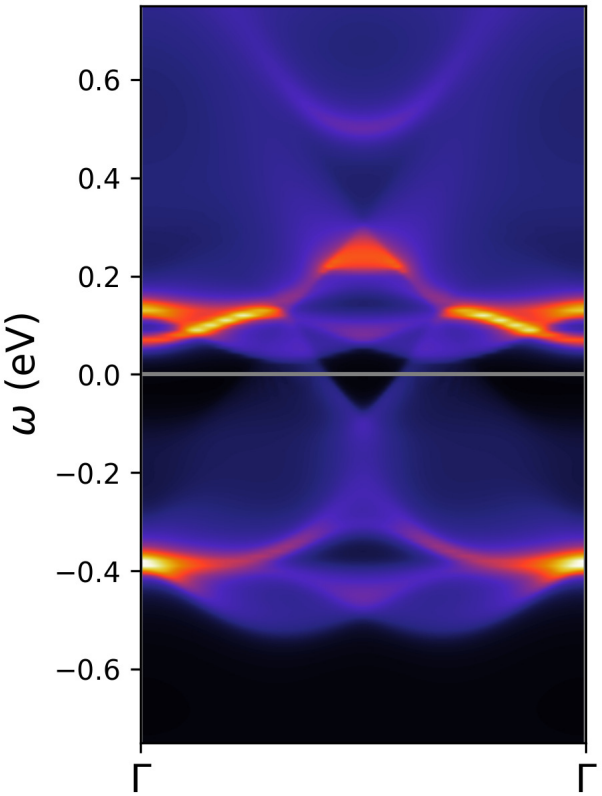

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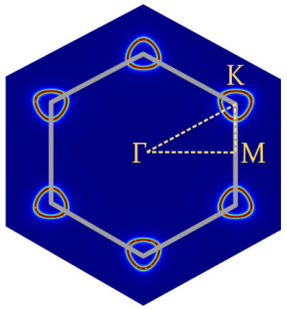
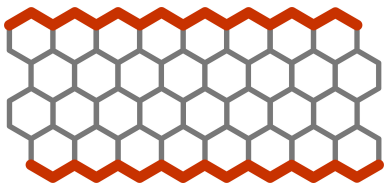
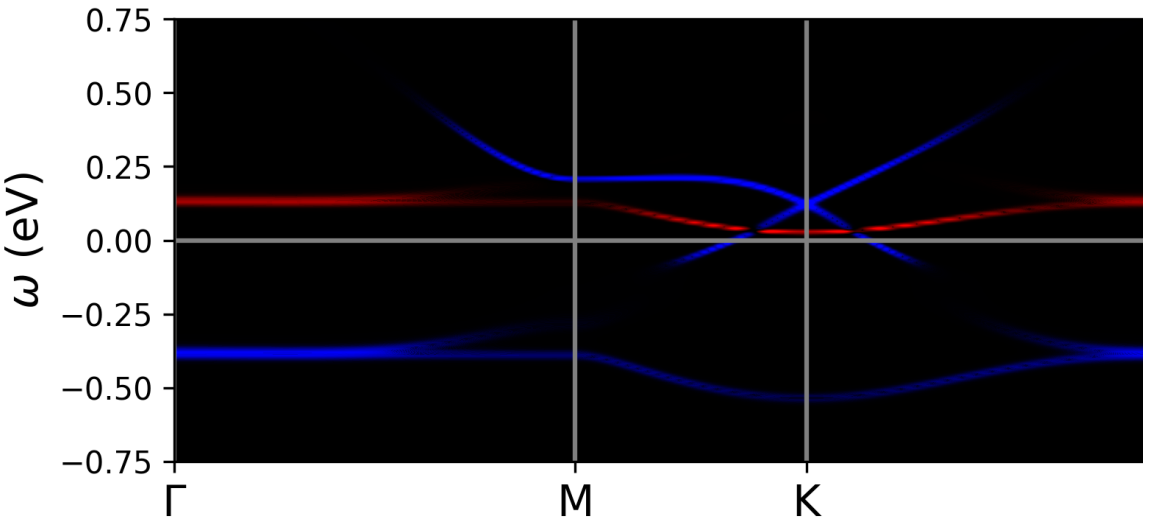
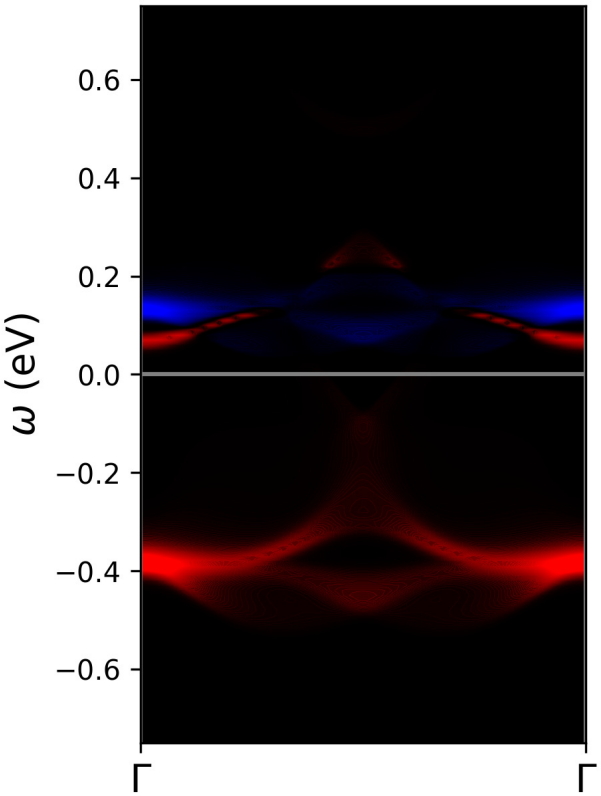




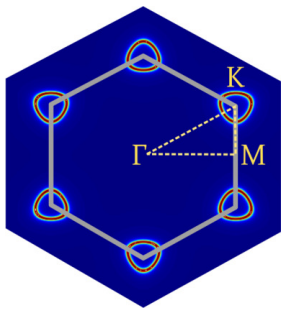
OJ and Karsten Held, PRB **98**, 115118 (2018)

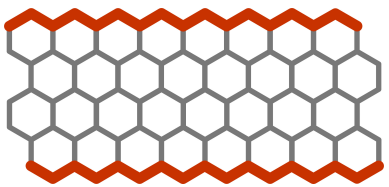
Ferromagnetic metallic (FM) phase





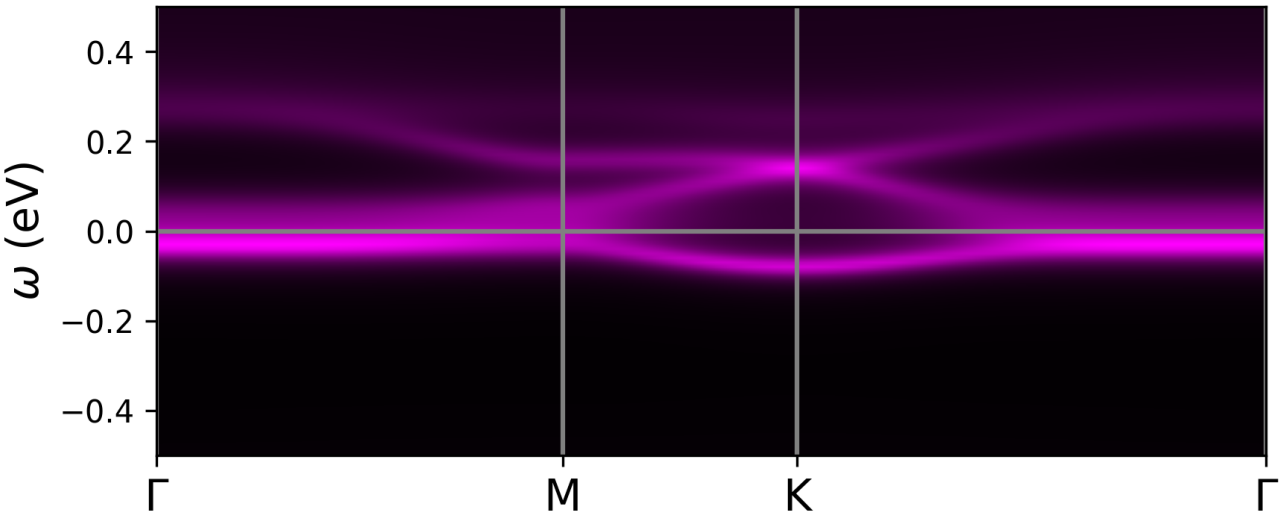
- Dirac point is not at the Fermi level
- large exchange splitting, sharp features
- Fermi surface differs from that of the non-interacting model
- edge states are visible in the unoccupied part of the spectrum



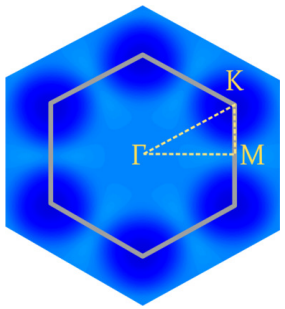


OJ and Karsten Held, PRB **98**, 115118 (2018)

Paramagnetic metallic (PM) phase



- strong renormalization
- broadening



OJ and Karsten Held, PRB **98**, 115118 (2018)

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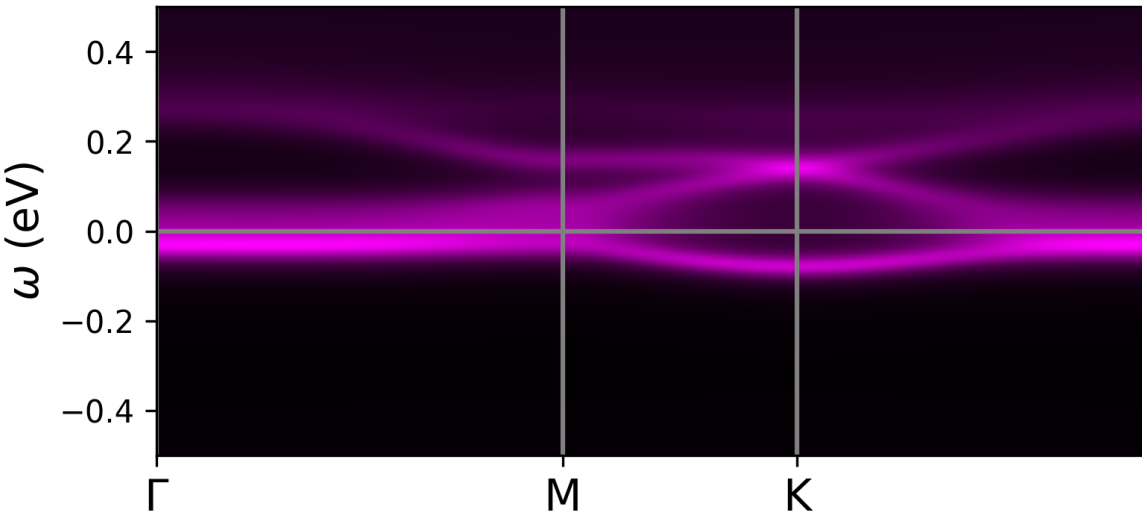
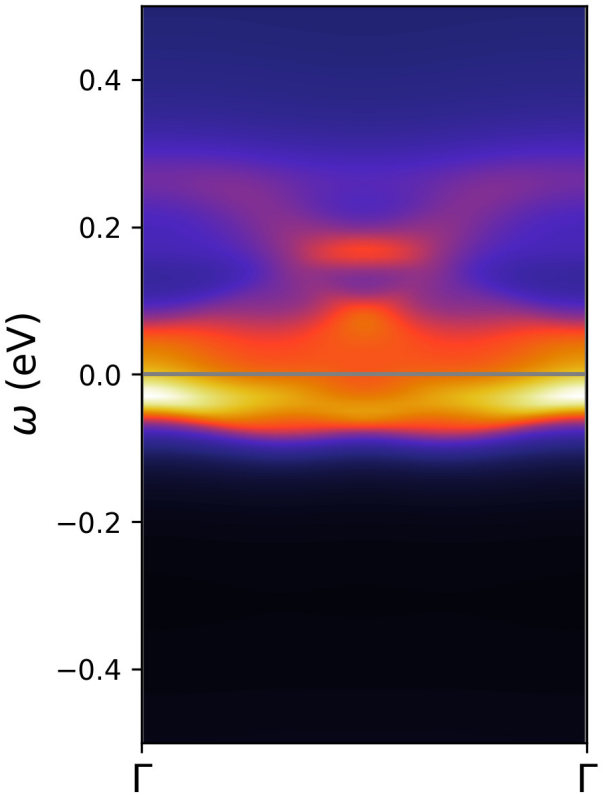
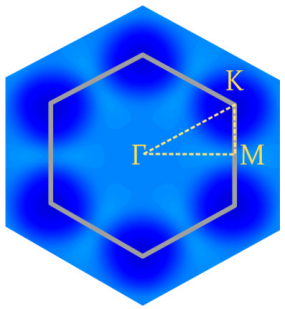
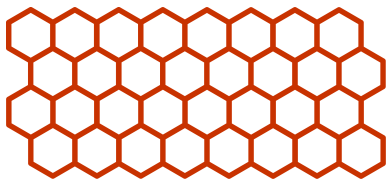




- strong renormalization
- broadening
- no edge states





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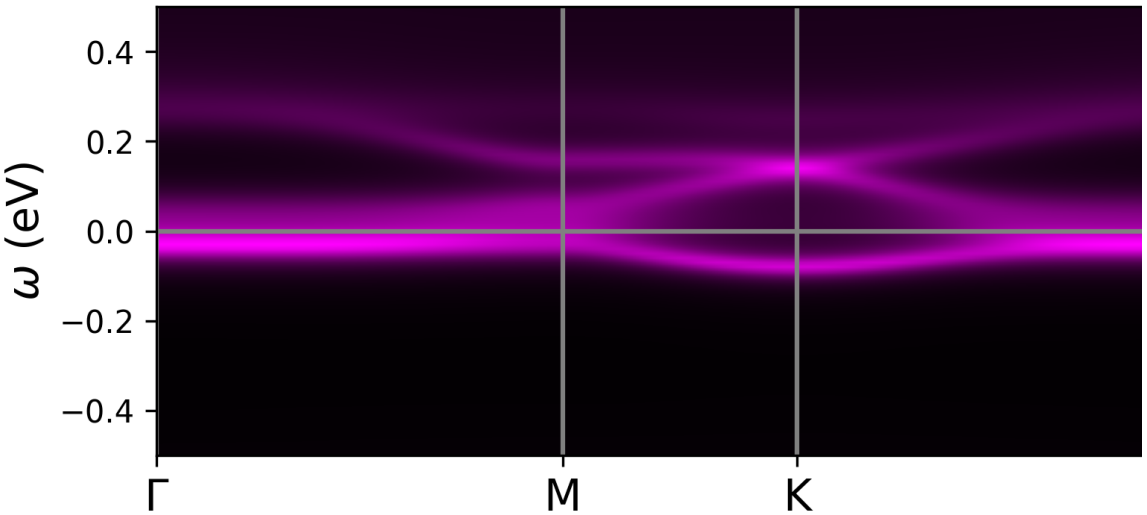

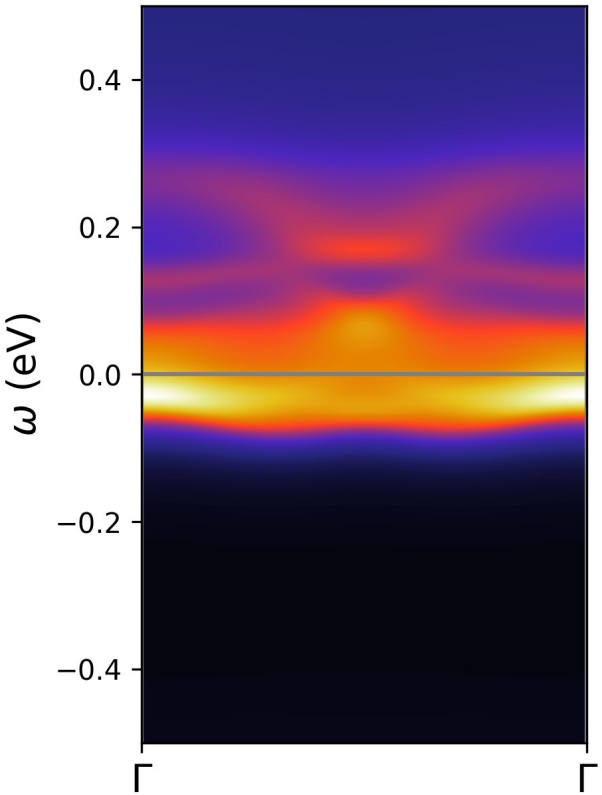

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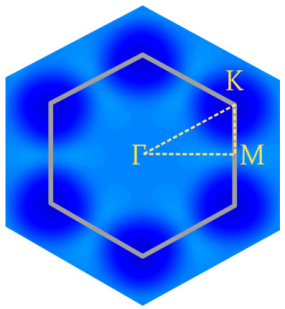
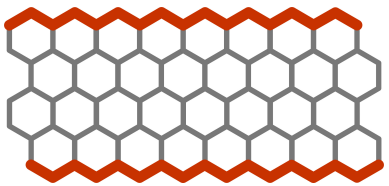
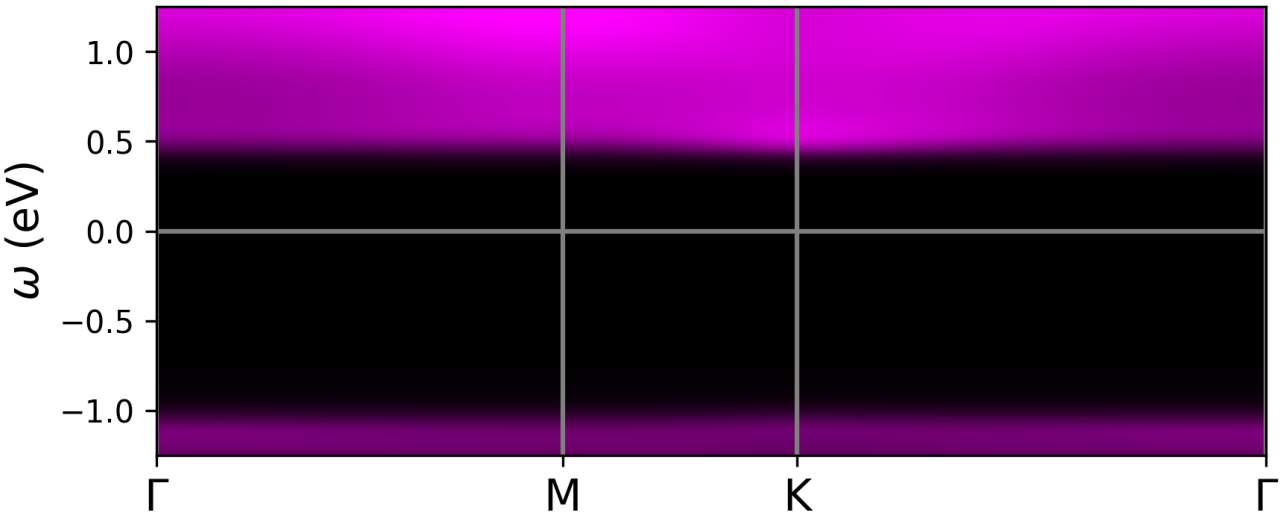


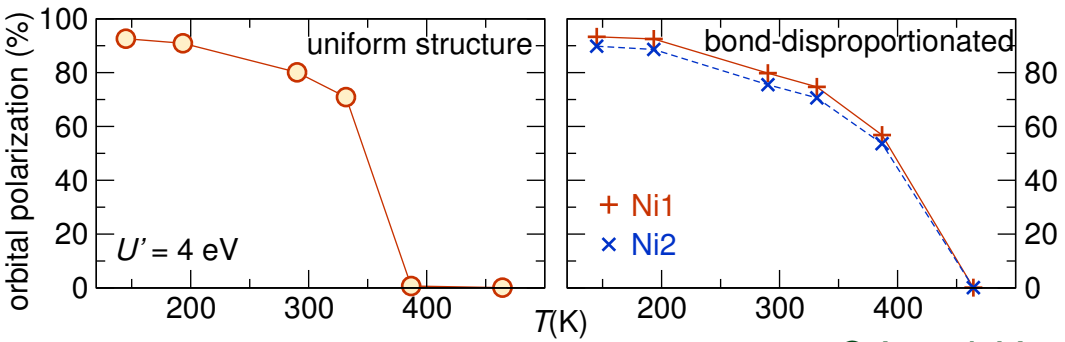


OJ and Karsten Held, PRB **98**, 115118 (2018)

Antiferro-orbitally-ordered insulating (AOI) phase



- only broad features
- sizable orbital polarization for both structures



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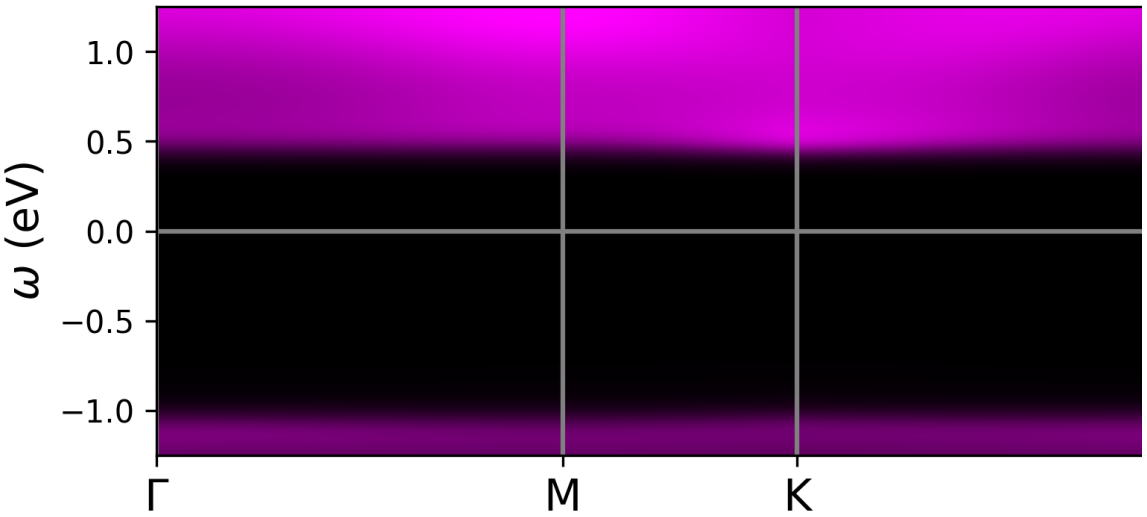

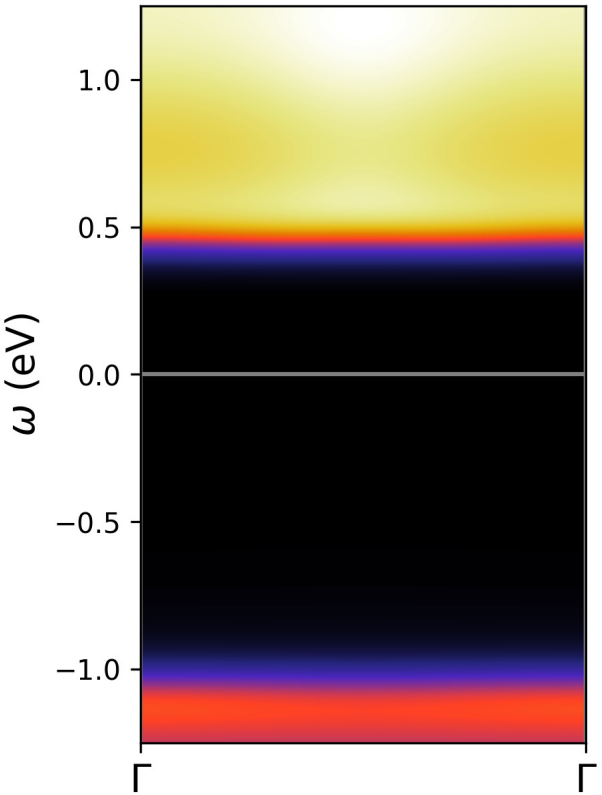

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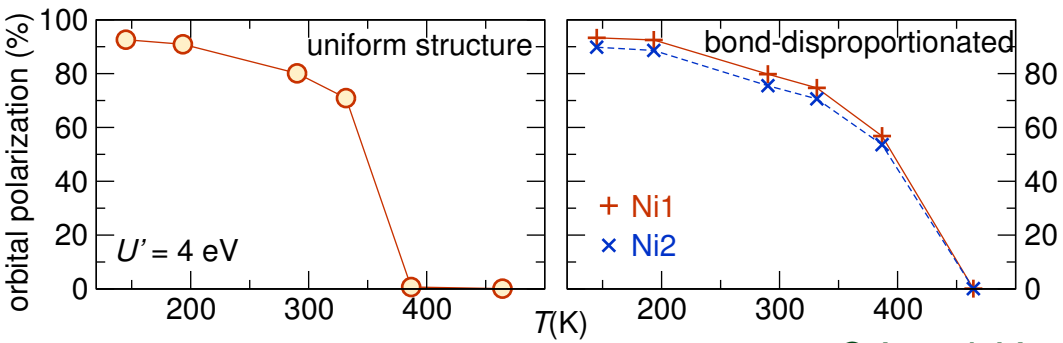

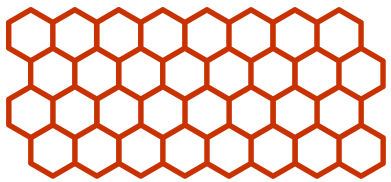

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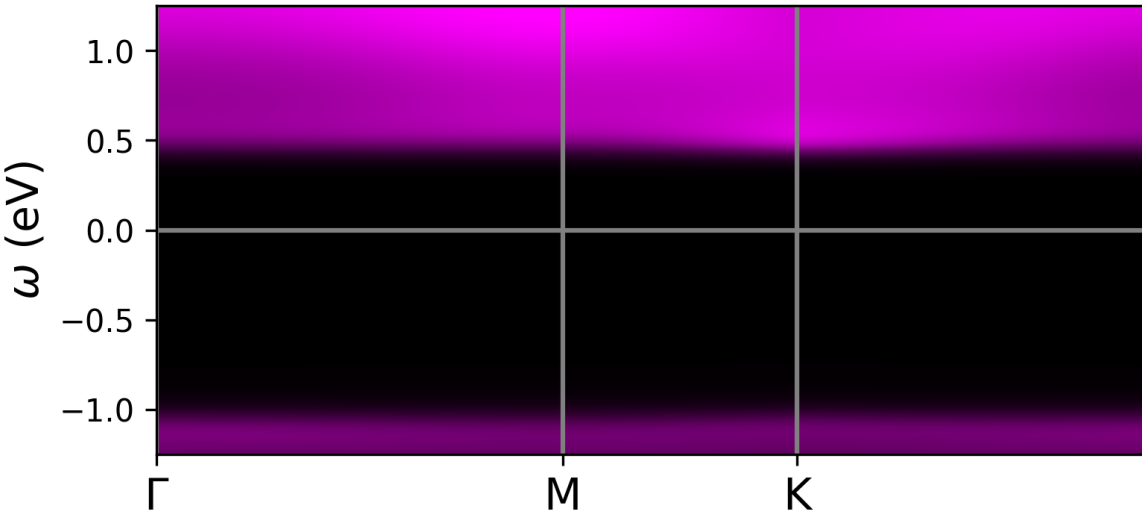

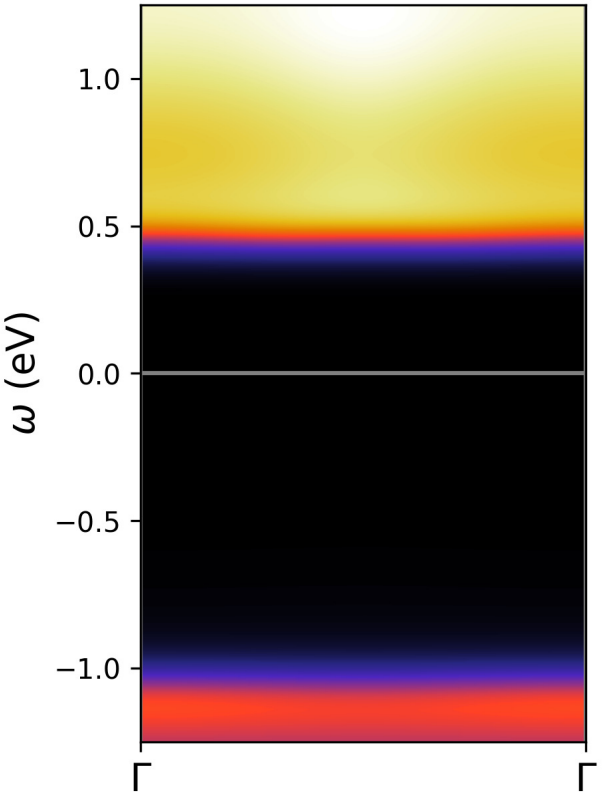

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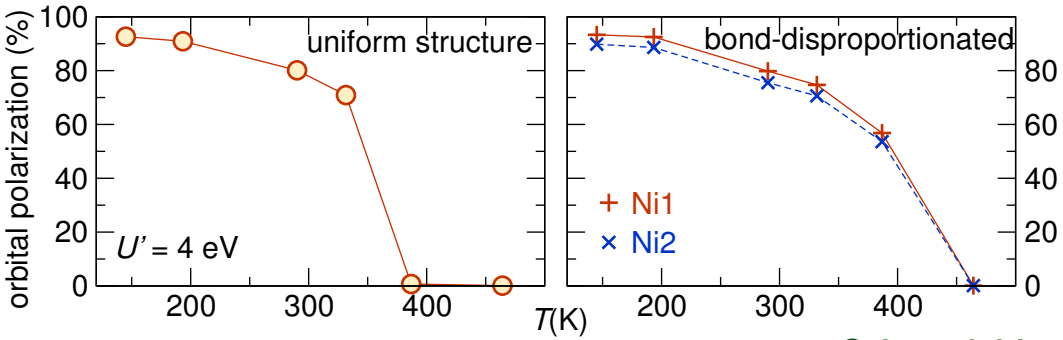
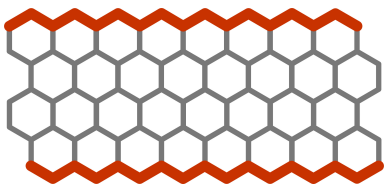
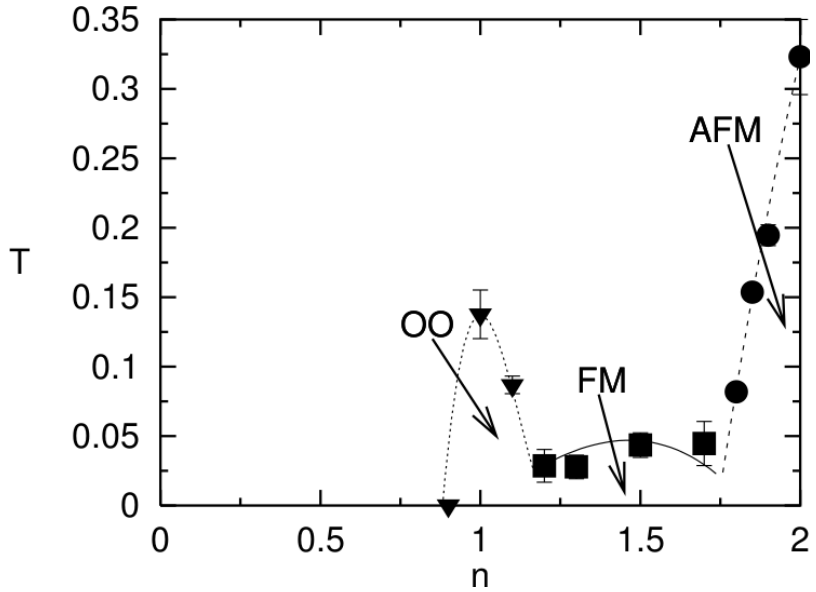




OJ and Karsten Held, PRB **98**, 115118 (2018)

Is it really that boring?

Similarities to the physics of a two-orbital Hubbard model?
Yes, a pronounced tendency towards ferromagnetism and **orbital ordering**



K. Held and D. Vollhardt, Eur. Phys. J. B **5**, 473 (1998)

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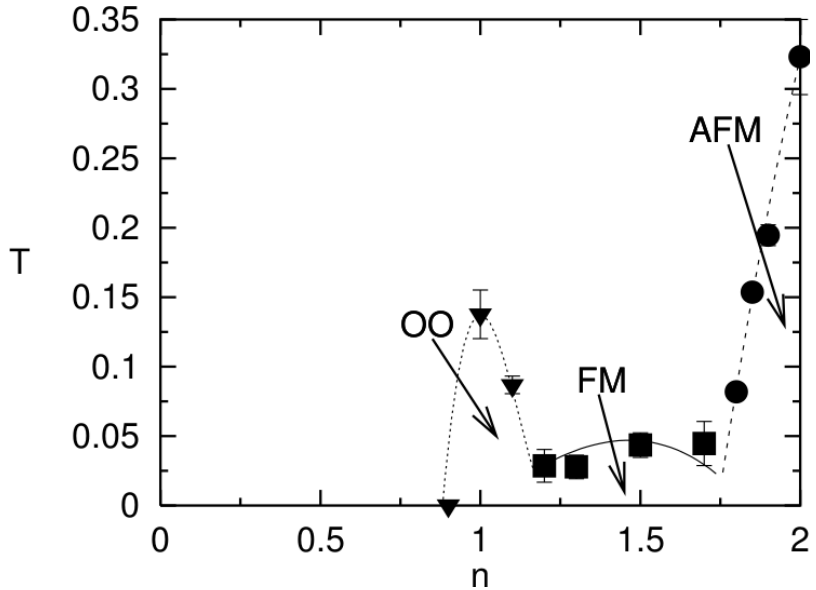
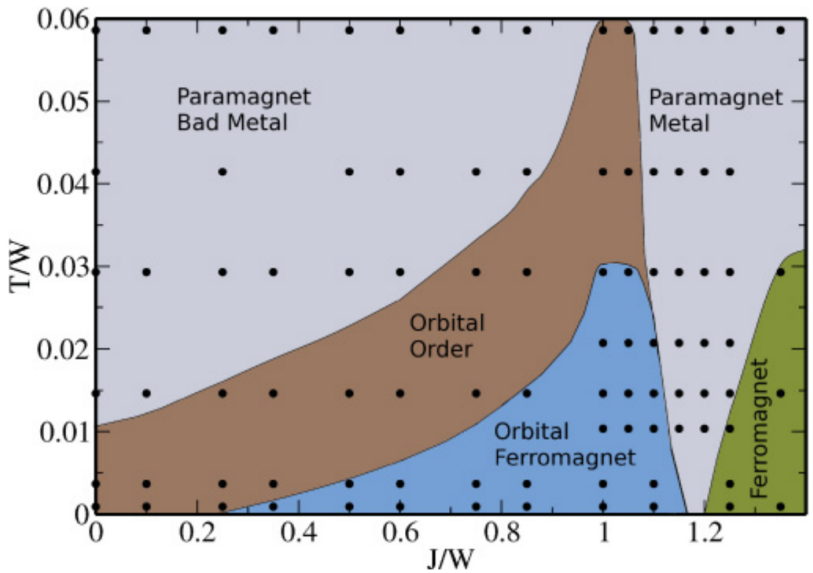
MIT between FM and ferromagnetic AOI
$\rightarrow$ **high magnetoresistance**



K. Held and D. Vollhardt, Eur. Phys. J. B **5**, 473 (1998)



R. Peters *et al.*, PRB **83**, 125110 (2011)

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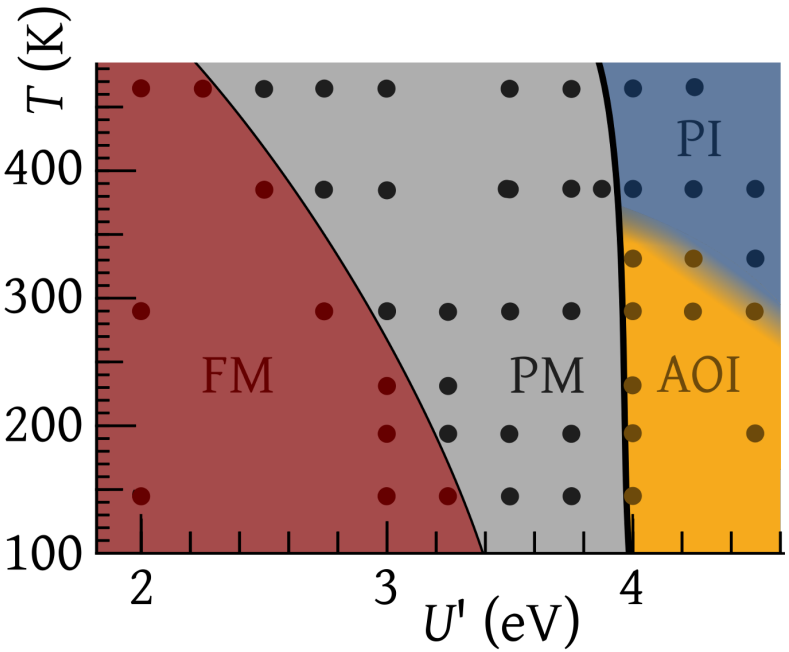

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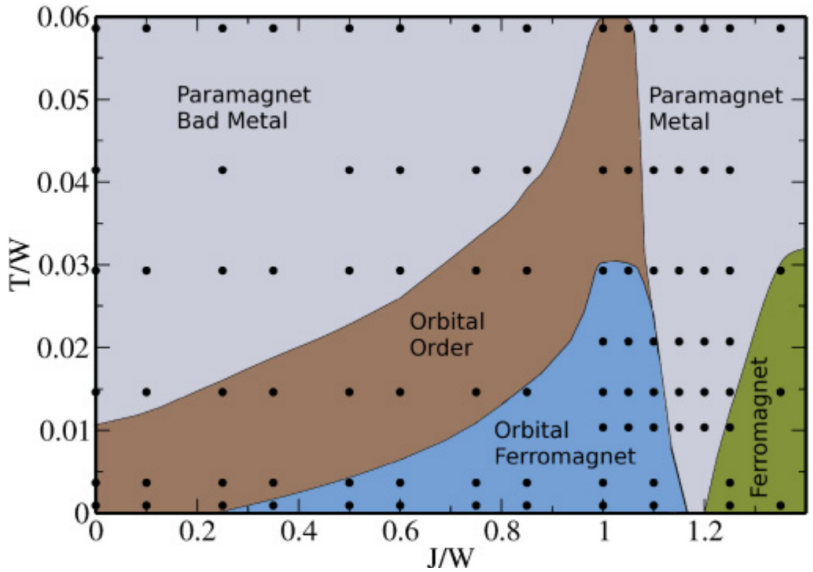
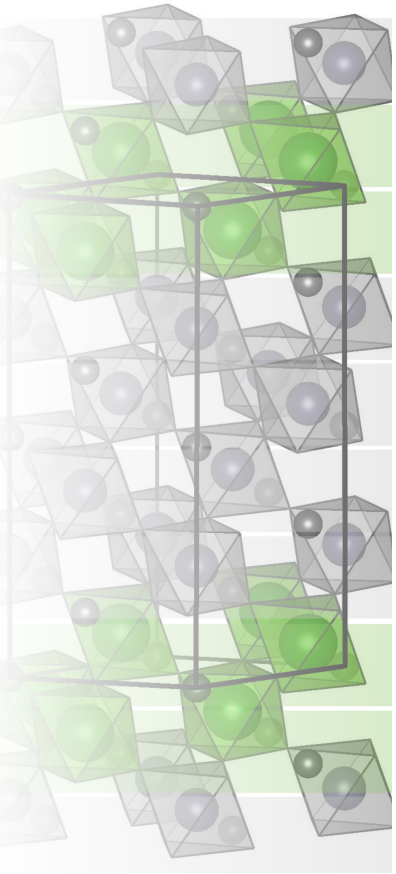
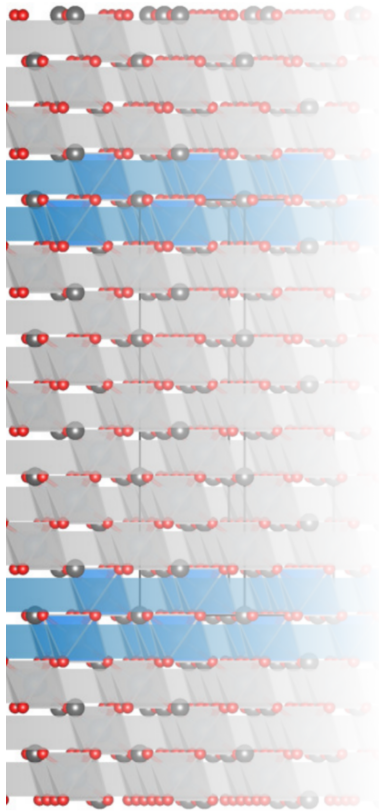


R. Peters *et al.*, PRB **83**, 125110 (2011)

Summary and Outlook



1. DFT+DMFT calculations for oxide heterostructures are feasible
2. $SrRuO_3 : SrTiO_3$
   - room temperature FM
   - QAH upon doping (different $4d$, different substrate)
3. $LaNiO_3 : LaAlO_3$
   - rich phase diagram, but no topological phases
   - possibly, high magnetoresistance at low temperatures
4. crystal structure matters



Outlook:

- precise structural information from experiment (distortions, rotations)
- extensions of DMFT (cluster, diagrammatic)

OJ, Z. Zhong, G. Sangiovanni, and K. Held, Dynamical mean field theory for oxide heterostructures (Springer Ser. Mater. Sci. **266**, 2018, pp. 215–243)

L. Si, OJ, G. Li, Z. Zhong, Z. Liao, G. Koster, and K. Held, PRL **119**, 026402 (2017)

OJ and K. Held, PRB **98**, 115118 (2018)