APS March Meeting

Electronic structure of RuO_2 under strain

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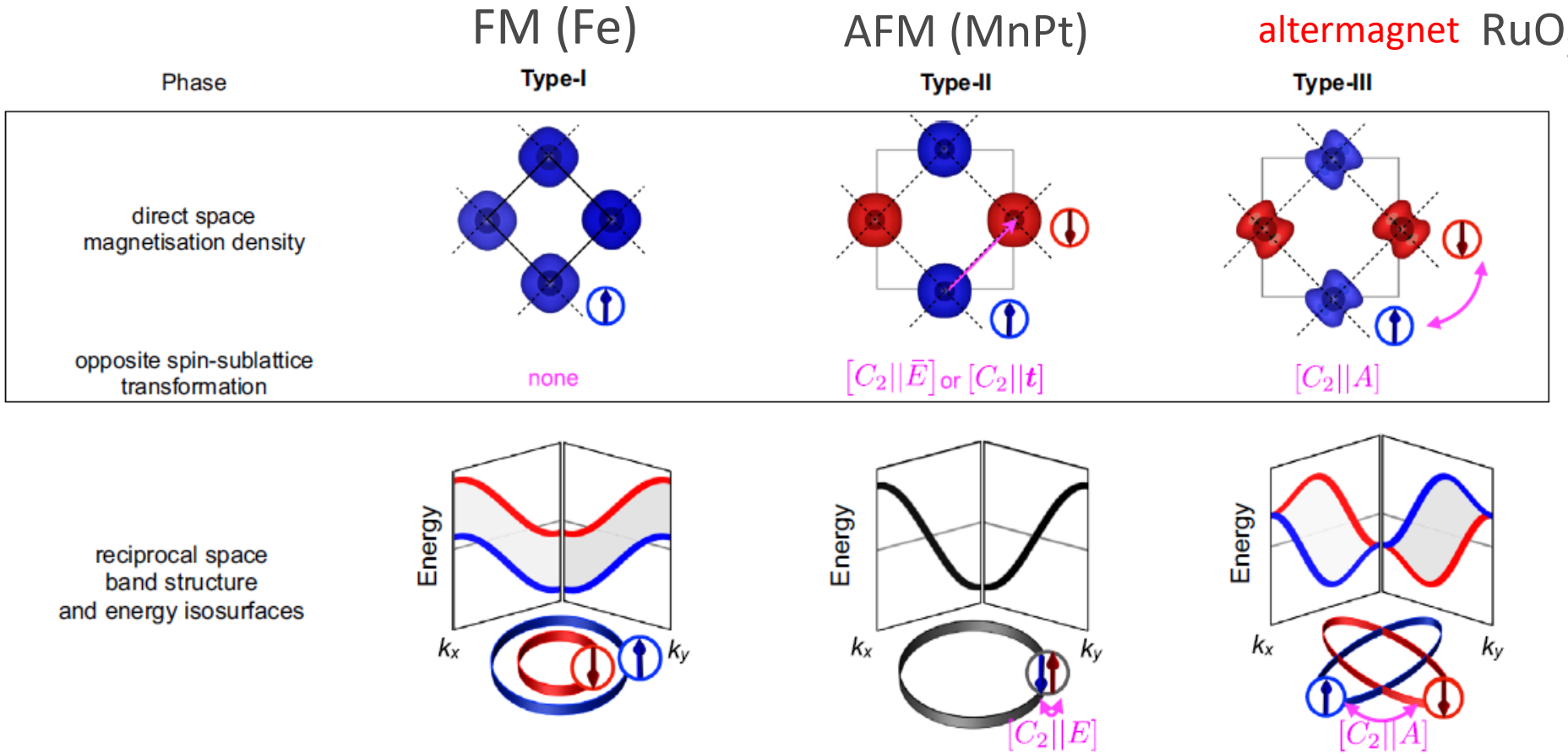
National Science Foundation MRSEC Materials Research Science and Engineering Centers

Center for Hybrid, Active, and Responsive Materials CHARM at the University of Delaware

ACCESS

RuO_2: a new type of magnetic material



Time-reversal symmetry	NO	YES	NO

Libor Šmejkal, Jairo Sinova, and Tomas Jungwirth, Phys. Rev. X 12, 031042 (2022)

Why strained RuO_2?

PHYSICAL REVIEW LETTERS **125,** 147001 (2020)

Editors' Suggestion | Featured in Physics

Superconductivity in Uniquely Strained RuO_2 Films

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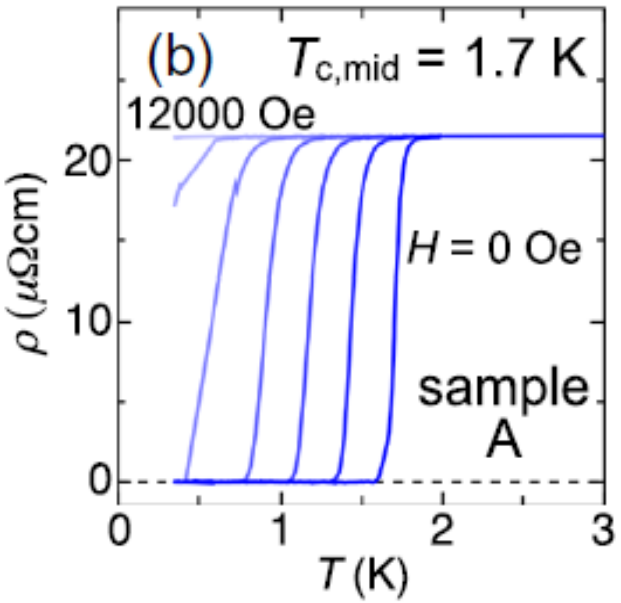
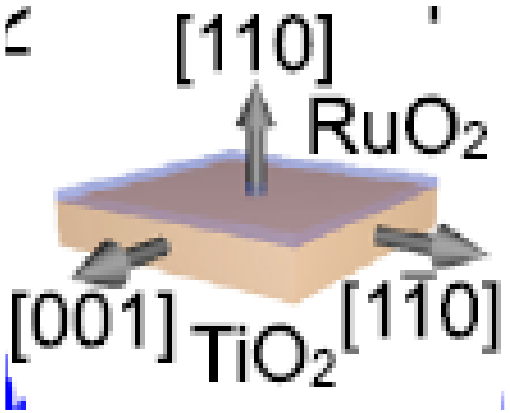




nature COMMUNICATIONS | NATURE COMMUNICATIONS | (2021)12:59 |

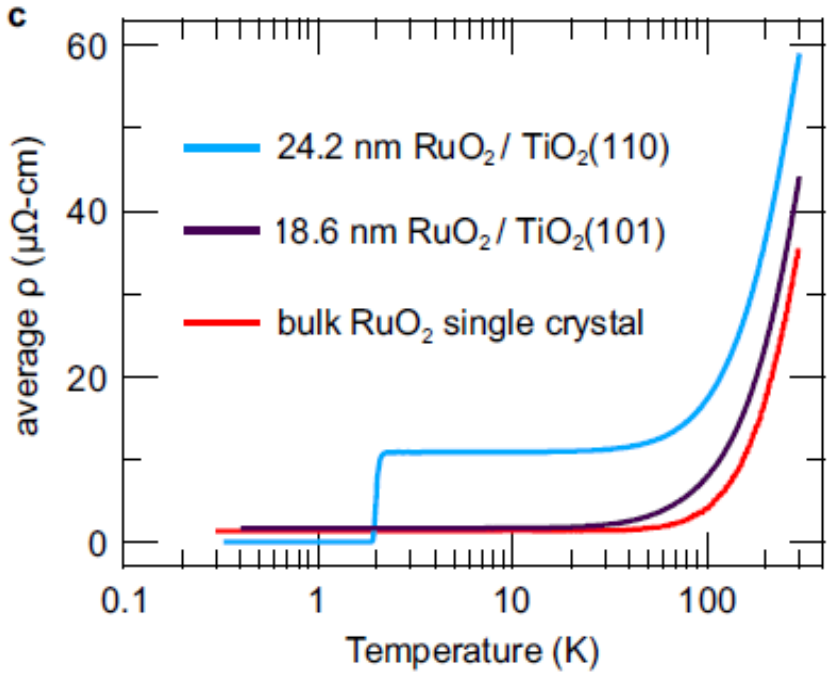
ARTICLE

https://doi.org/10.1038/s41467-020-20252-7 OPEN

Check for updates

Strain-stabilized superconductivity

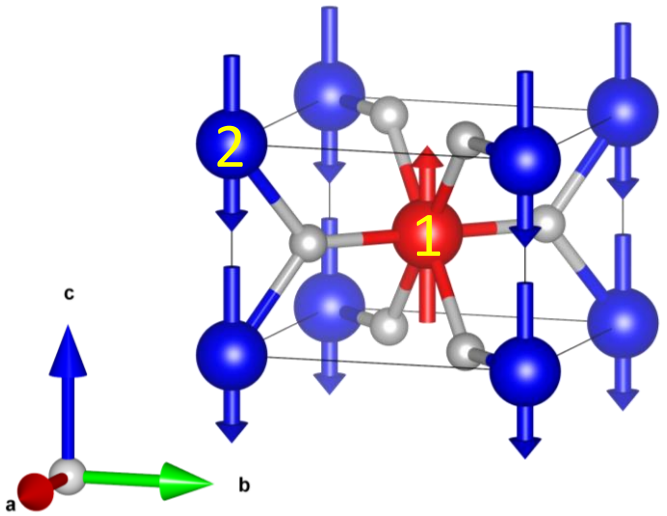
J. P. Ruf[1✉], H. Paik[2,3], N. J. Schreiber[3], H. P. Nair[3], L. Miao[1], J. K. Kawasaki[1,4], J. N. Nelson[1], B. D. Faeth[1,2], Y. Lee[1], B. H. Goodge[5,6], B. Pamuk[5], C. J. Fennie[5], L. F. Kourkoutis[5,6], D. G. Schlom[3,6,7] & K. M. Shen[1,6✉]

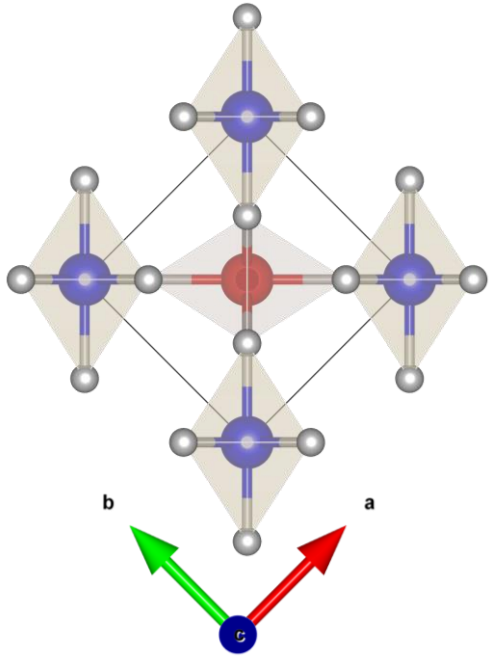


Masaki Uchida et al., Phys Rev Lett **125**, 147001 (2020)

Ruf, J.P., Paik, H., Schreiber, N.J. et al. Strain-stabilized superconductivity. Nat Commun **12**, 59 (2021)

Computational Methods





- First principles DFT
- VASP package: PW basis set + PAW potential
- Wannier90 for very dense k-mesh quantities

GGA, GGA+U, META-GGA, hybrid functional?

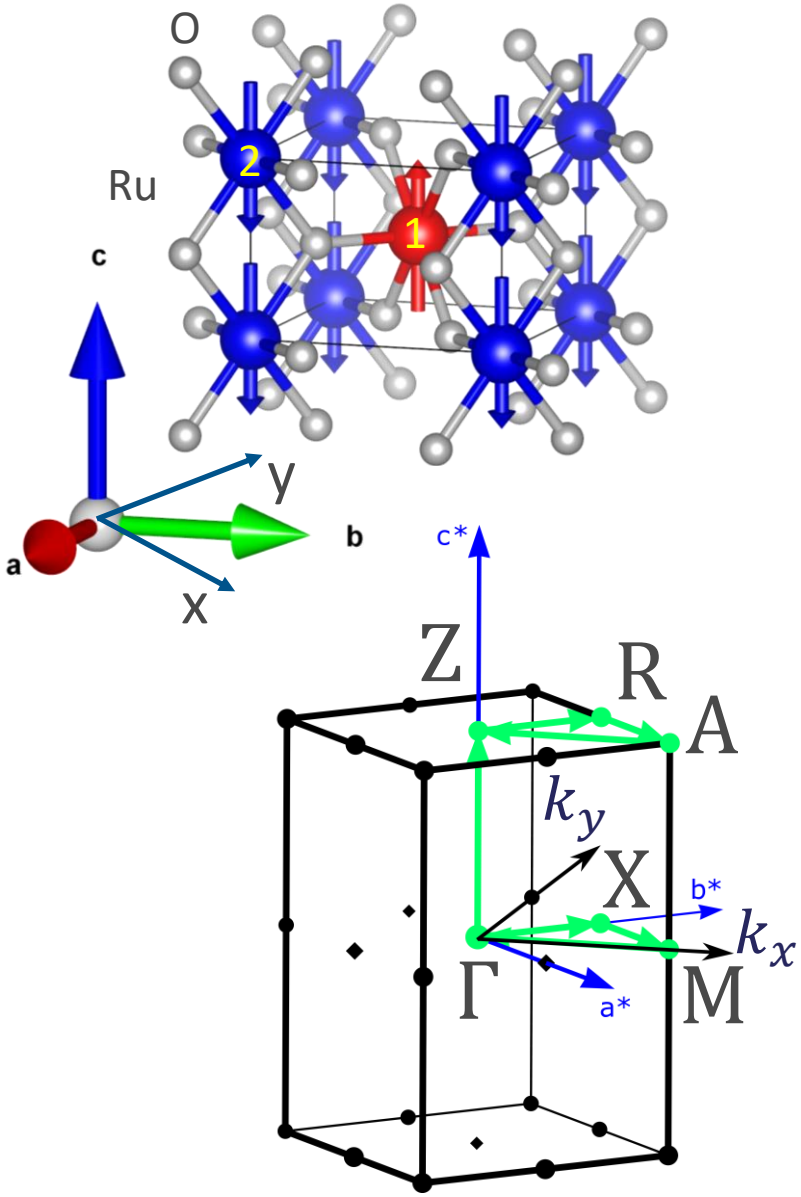
Testing parameters:

- 600 eV ENCUT
- 12x12x18 k-point mesh
- Force convergence criteria: 0.001 eV/Å

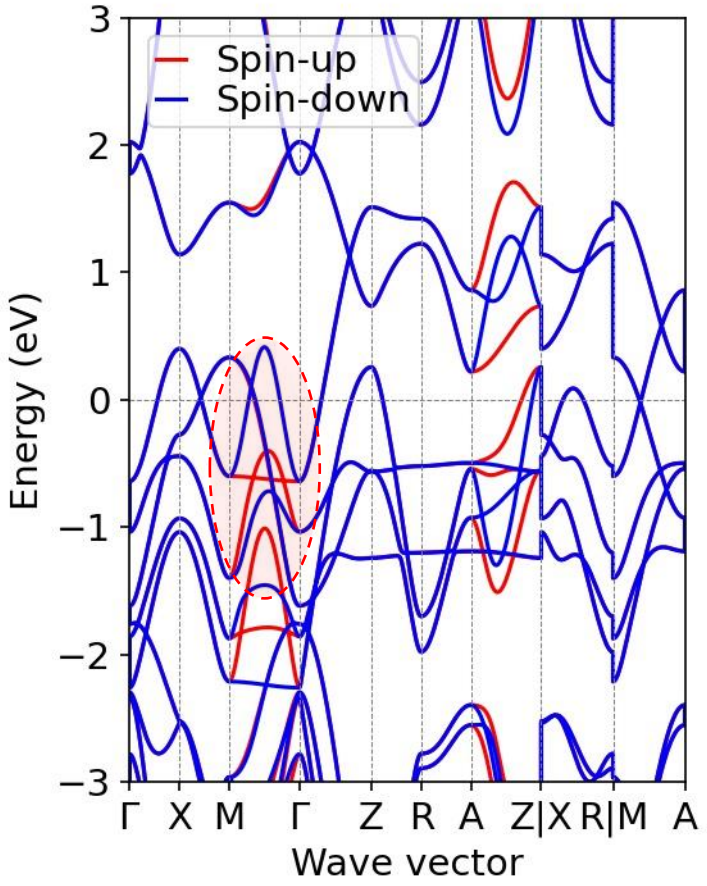
- PBE: non-magnetic
- HSE06: semiconductor
- PBE+U: not very good lattice constant
- SCAN: good lattice constants, magnetic moment and electronic structure

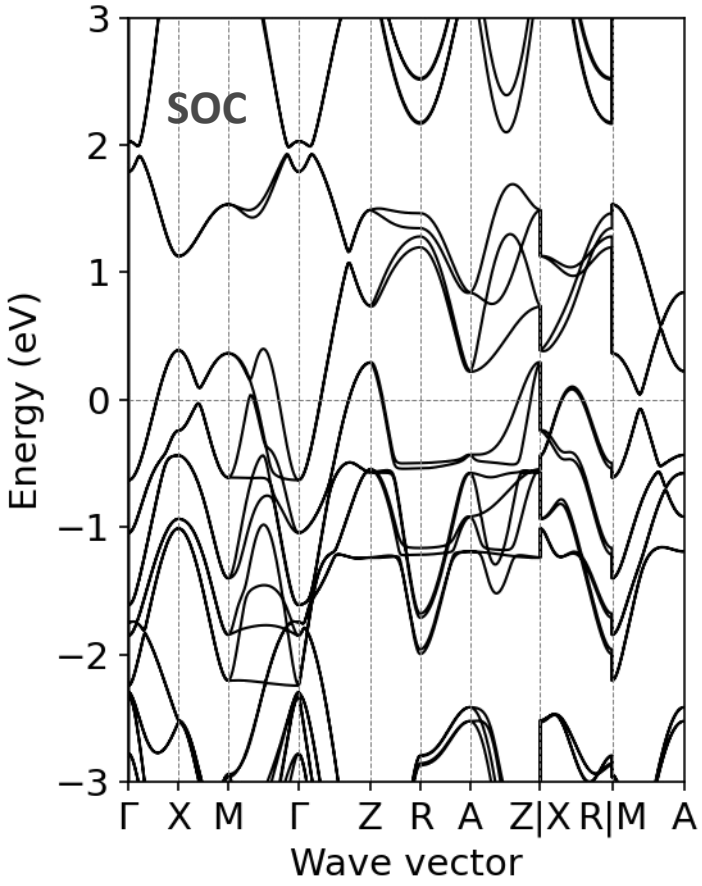
Method	a (Å)	c(Å)	Local moment (μB)
PBE	4.522	3.121	0.005
PBE+U (1.0)	4.519	3.126	0.005
1.25	4.532	3.130	0.848
1.5	4.538	3.133	0.996
2.0	4.549	3.136	1.205
SCAN	4.491	3.111	1.024
experiment	4.490	3.110	Varied 0.2 ~ 1

Electronic structure of bulk RuO_2



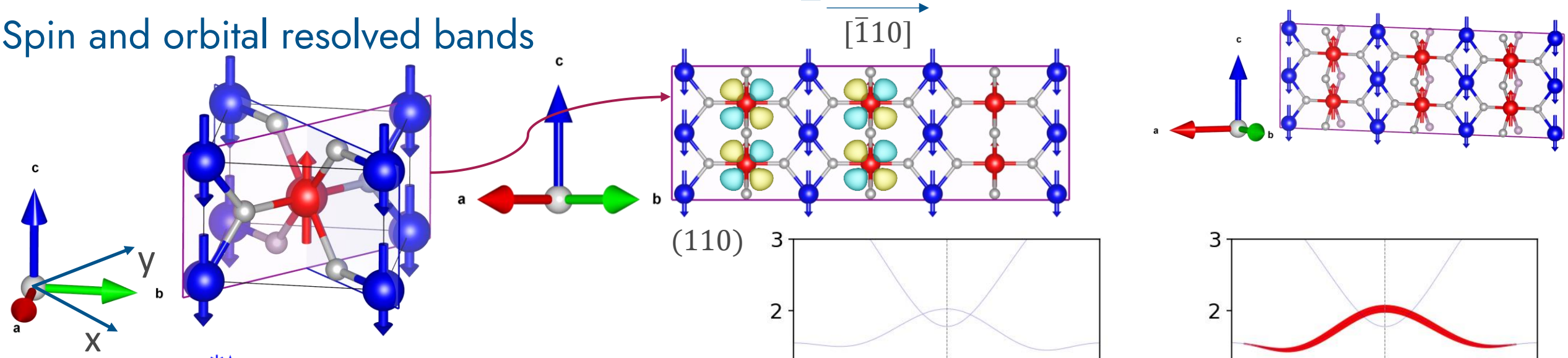
- Metallic collinear AFM
- Large spin polarization along ⟨110⟩
- SOC has little effect



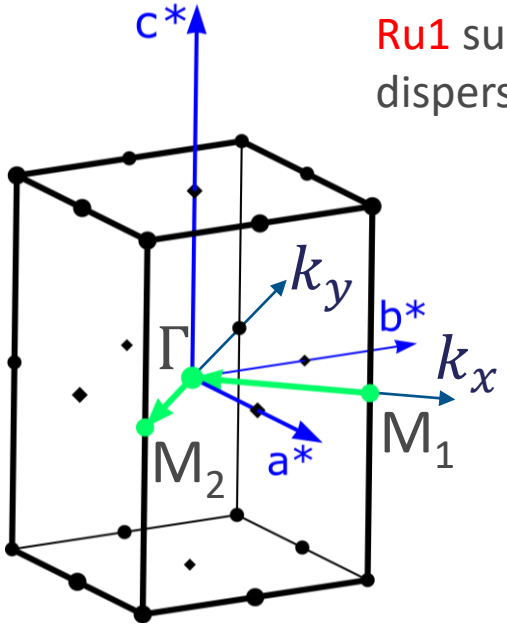


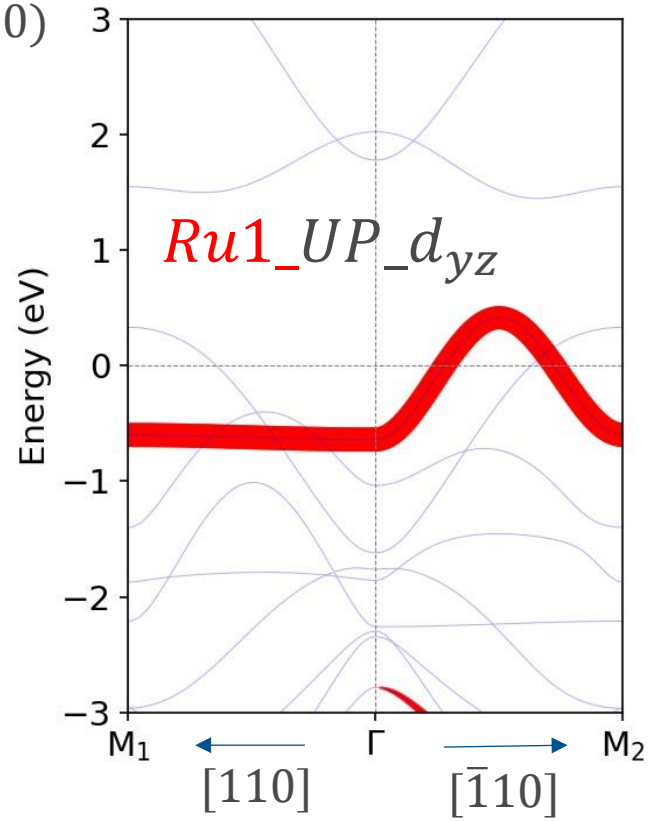
Electronic structure of bulk RuO_2

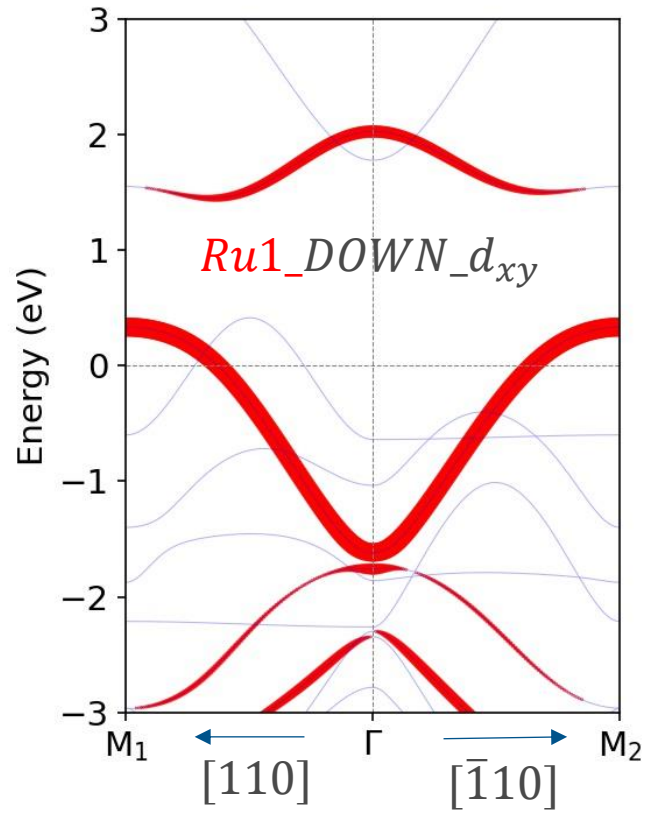
Spin and orbital resolved bands



Ru1 sublattice (in red) defines dispersion along $[\bar{1}10]$

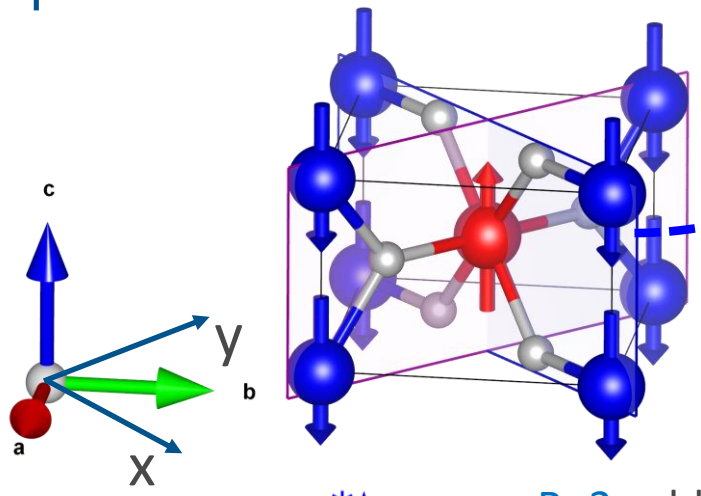


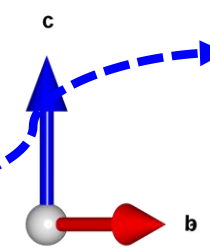


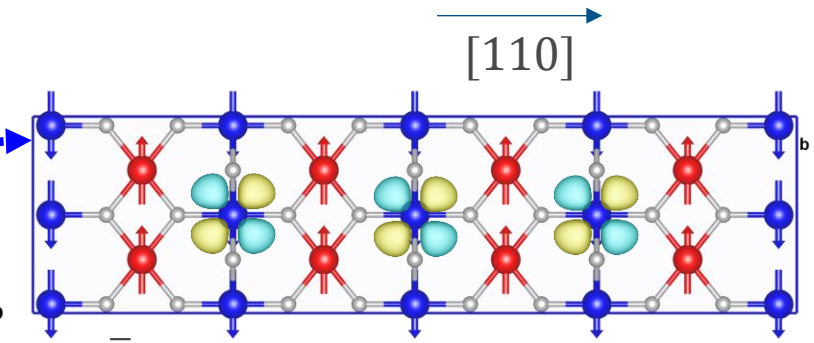


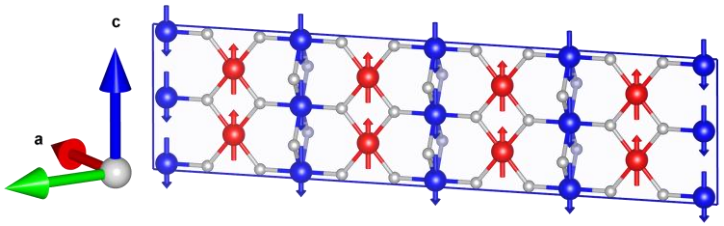
Electronic structure of bulk RuO_2

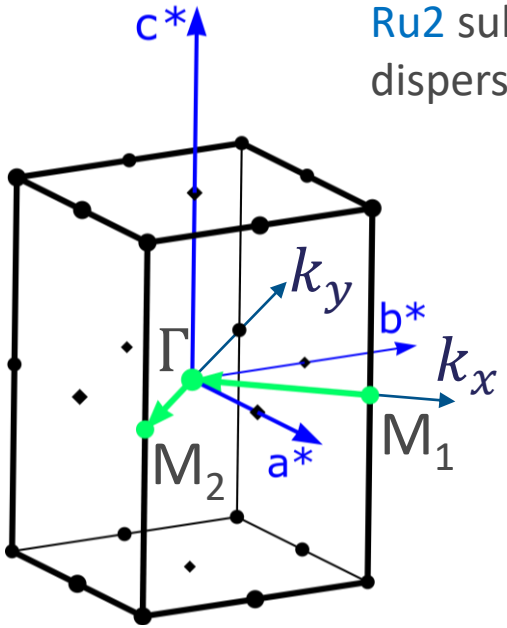
Spin and orbital resolved bands



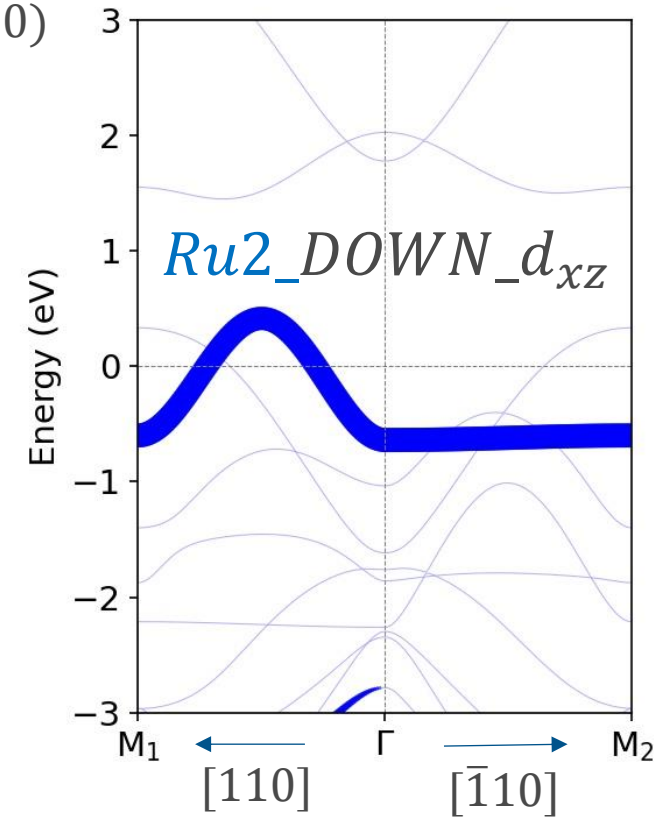


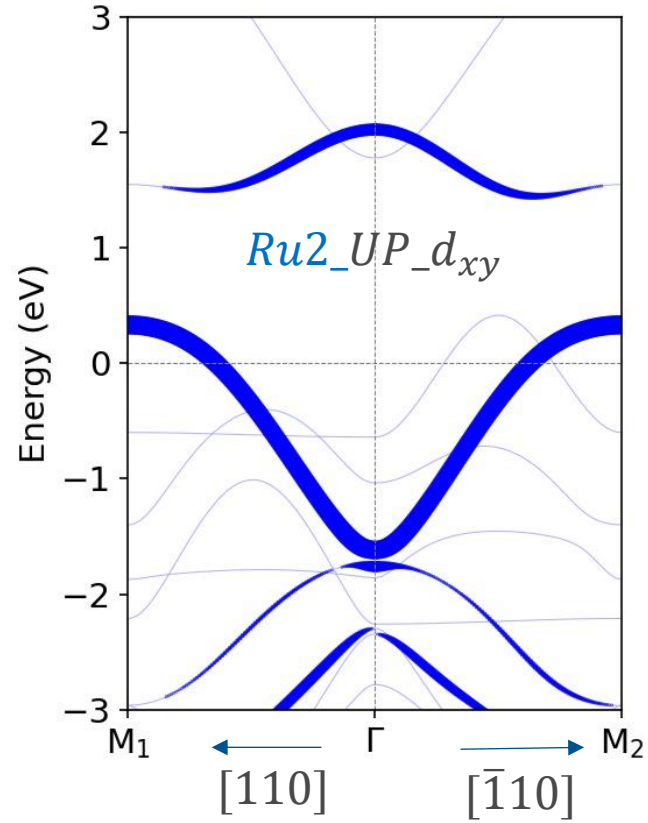






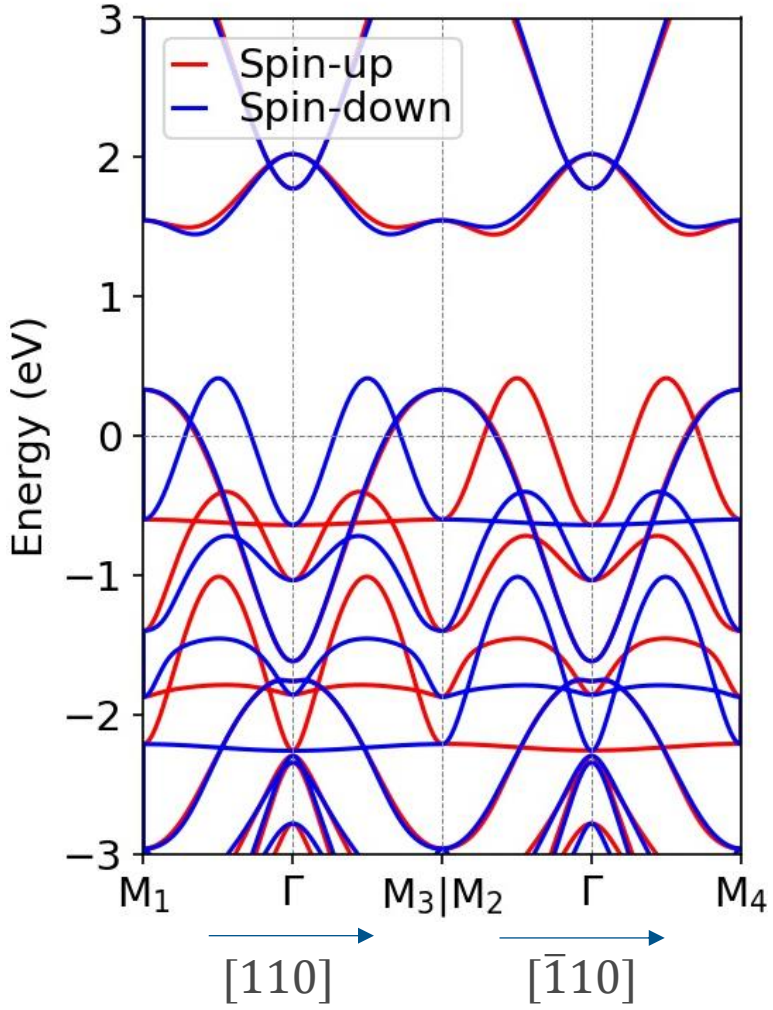
Ru2 sublattice (in blue) defines dispersion along [110]



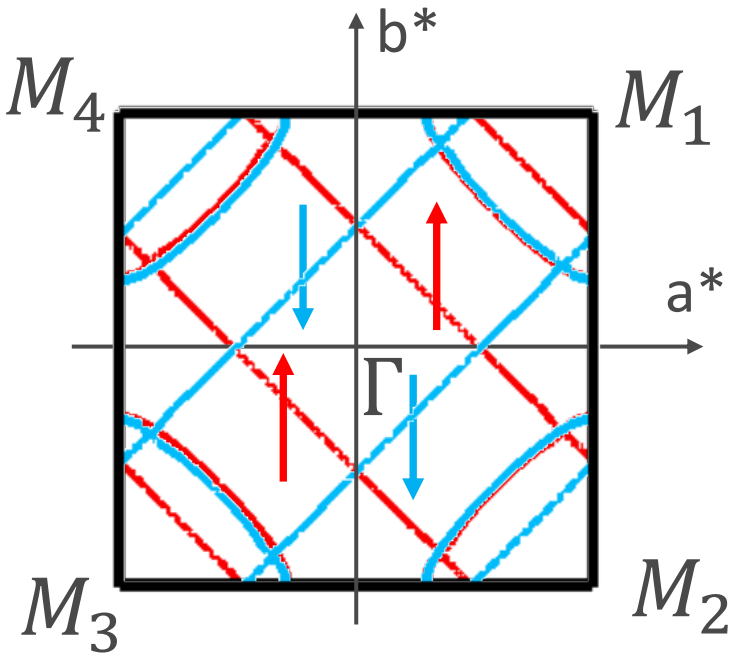


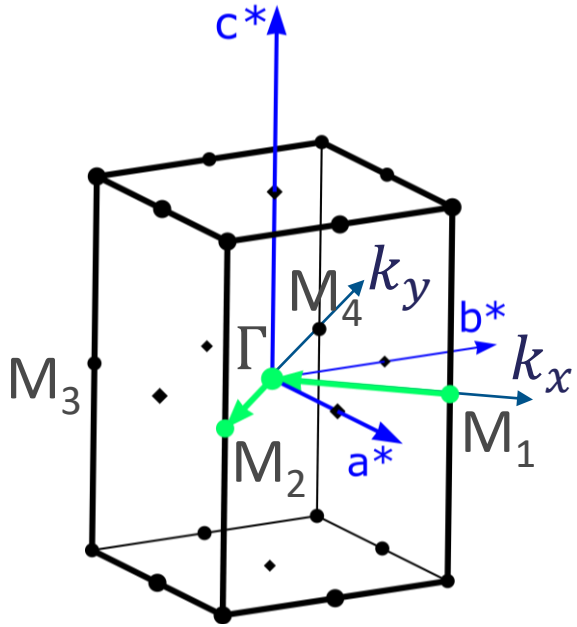
Electronic structure of bulk RuO_2

Closer look at the directions with large spin polarization



Fermi surface at $k_z = 0$





How to break the symmetry in ab-plane?

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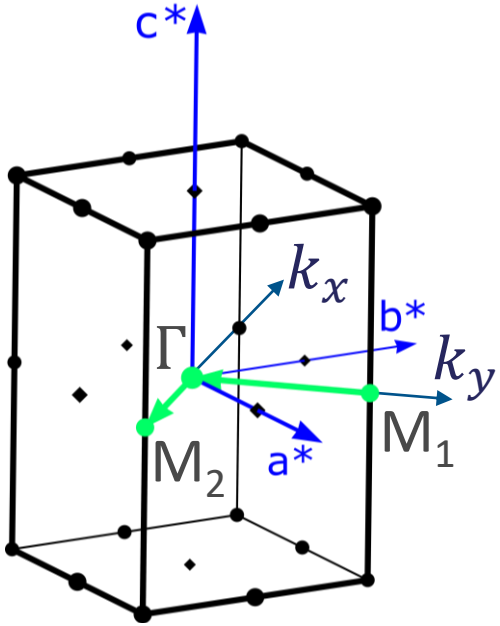
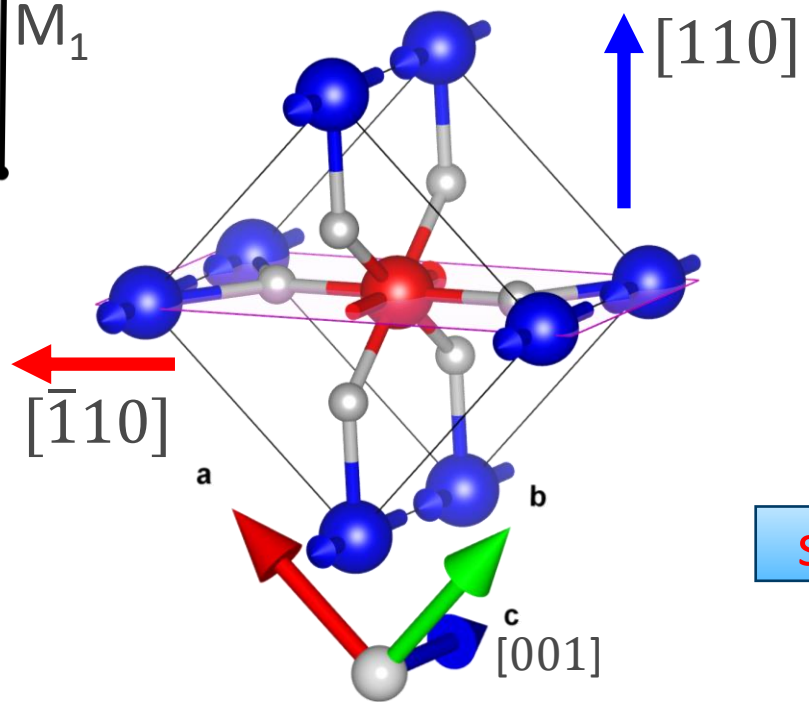
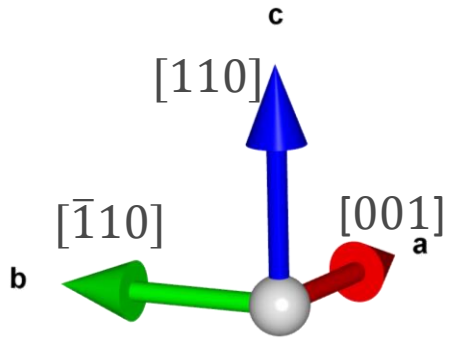
Strained RuO_2 with growth direction along [110]

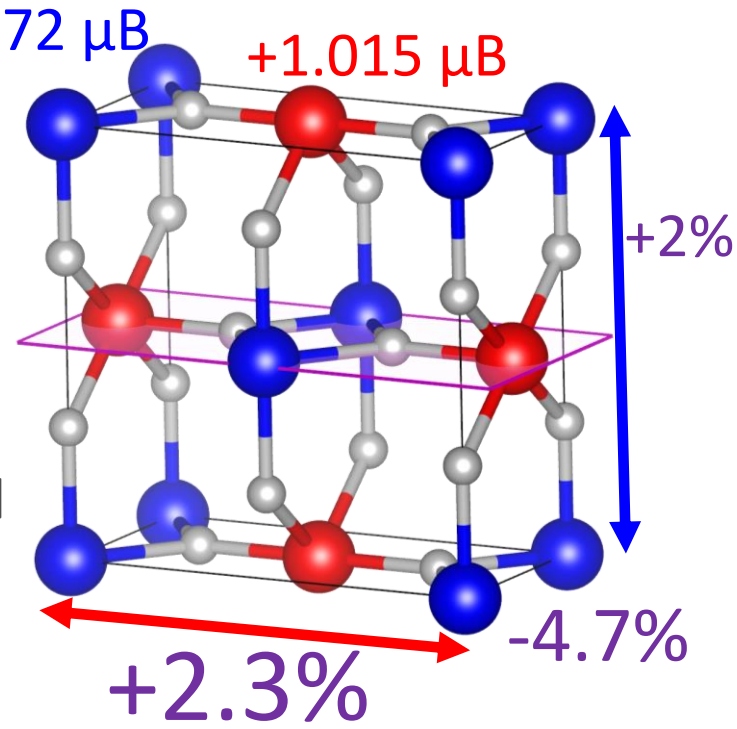


Net magnetization of ~0.2 μB per unit cell
Spin moments lying along the original easy axis



strain





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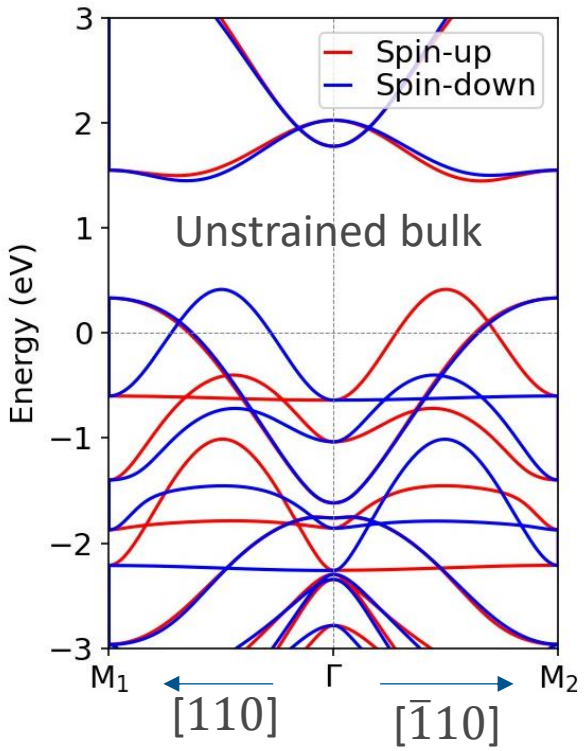
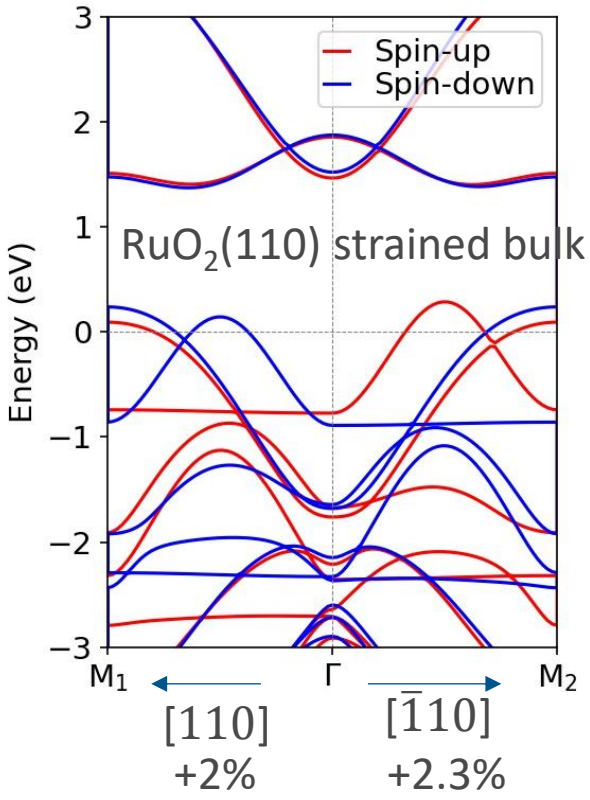
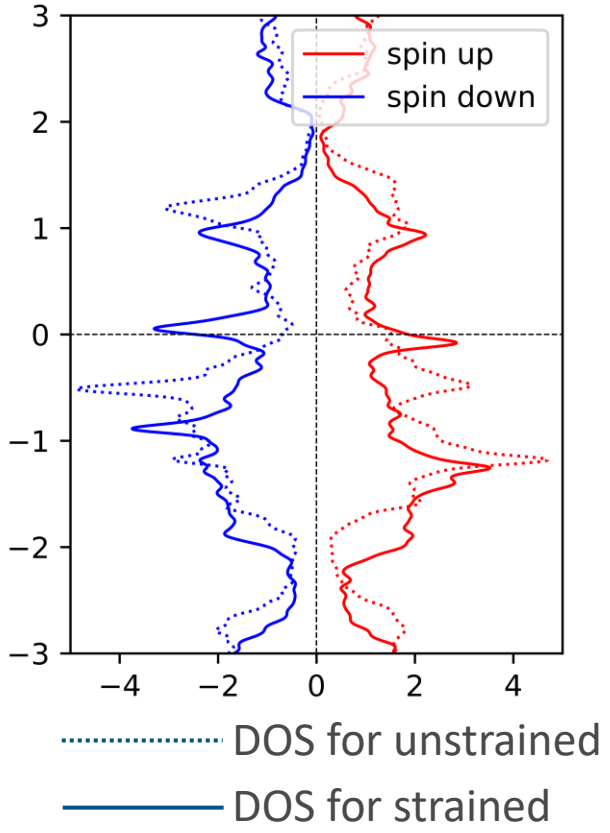
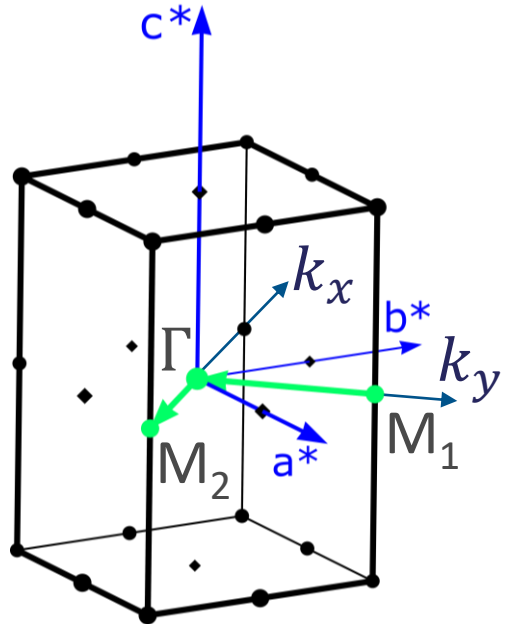
Electronic structure of strained vs unstrained RuO_2

Strain induces a net magnetization with high density of states close to Fermi level









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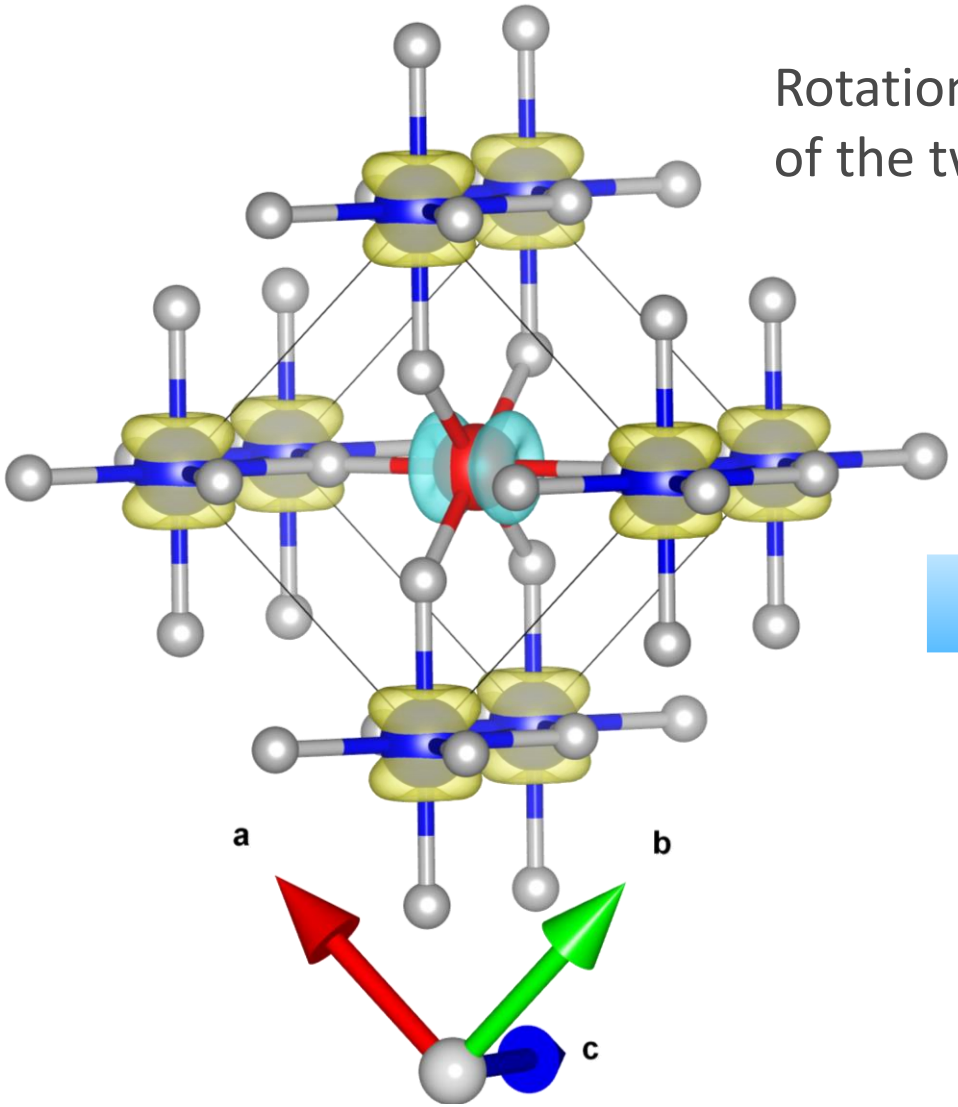
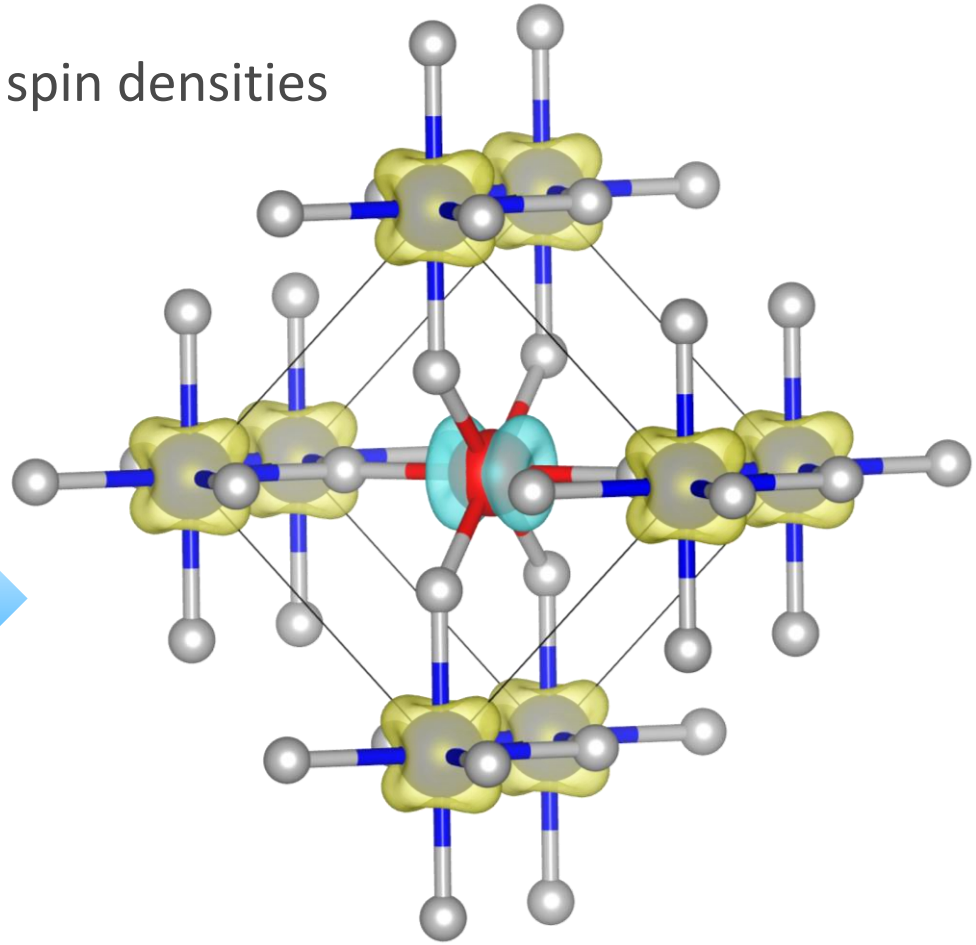
Magnetization density: symmetry breaking



Rotational symmetry connecting spin densities of the two sublattices broken

Applying strain



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Conclusion and future study

- Electronic structure of RuO_2 can be tuned by strain engineering
- Under strain, crystal symmetry broken leading to a net magnetization and higher DOS near E_F

  - Effect of strain in thin films
  - TRS broken induced responses of the materials