

Optimization of strain-induced superconductivity in RuO₂ enabled by physics-informed surrogate models

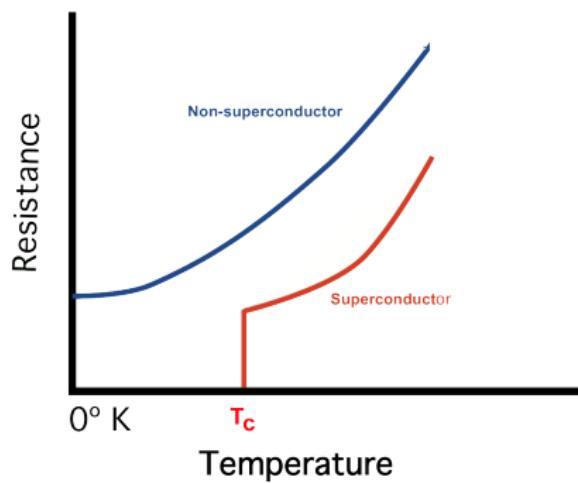
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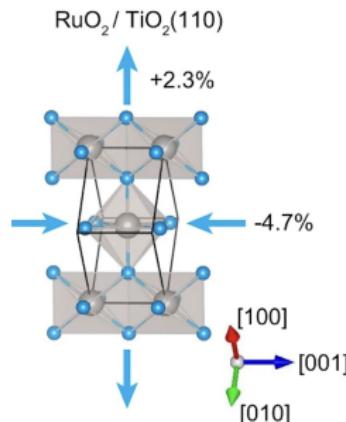
Superconductivity

- Conductance with *zero* electric resistance.
- Used in quantum computing, astronomical tools, etc.



Strain-induced superconductivity in RuO₂

- RuO₂ is normally not superconducting.
- Consider so-called RuO₂/TiO₂(110) strain.
- Observe superconductivity with $T_c \approx 2\text{ }^{\circ}\text{K}$ ¹



¹Ruf, J.P., Paik, H., Schreiber, N.J. et al. Strain-stabilized superconductivity. Nat Commun 12, 59 (2021).

Density Functional Theory (DFT): numerical simulation of material properties to explain and search for strain-induced superconductivity

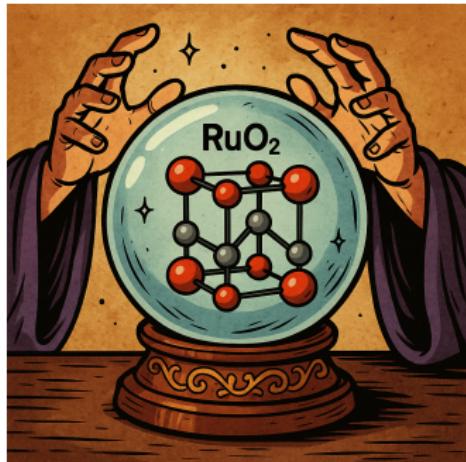


Figure: DFT allows us to “see inside” RuO_2 .
(ChatGPT 4o)

- DFT explains superconductivity in $\text{RuO}_2/\text{TiO}_2(110)$.
- Ongoing research: prediction and subsequent observation of strain-induced superconductivity in $\text{RuO}_2/\text{TiO}_2(100)$.^a

^aPamuk, B., Wadehra, N., Kaldybayev R., et al. Strain-dependent superconductivity in RuO_2 . APS Global Summit Abstracts, Session MAR-W23, (2025).

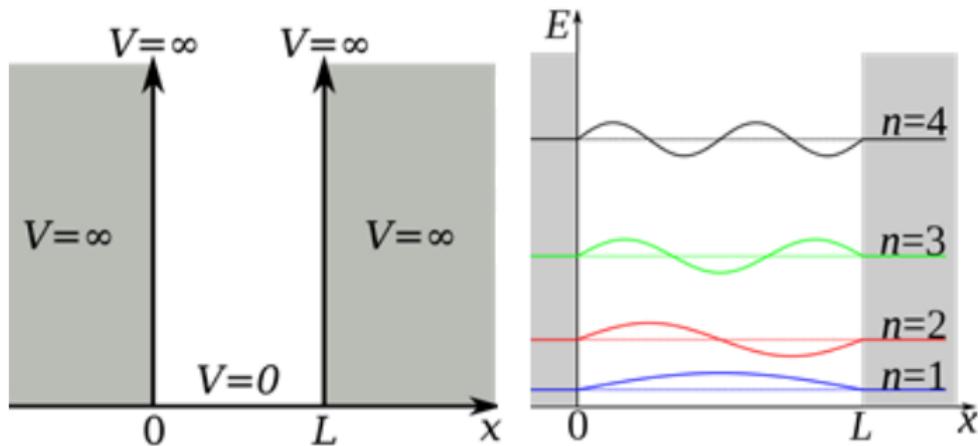
My goal: use surrogate models to perform a systematic and exhaustive search for superconductivity-inducing strains

- What strains are the best for superconductivity?
- Way too many possible strains to examine individually.
- My approach: train approximate models from some DFT data.



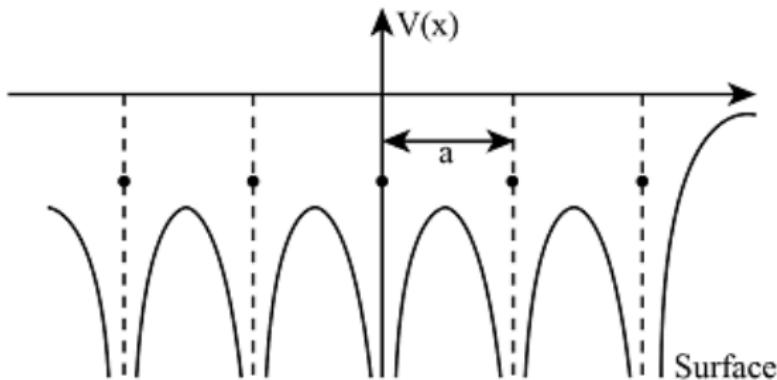
Superconductivity

1D Particle in a box



- Square well potential.
- Inside: $\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi = E\psi$.
- Outside: $V = \infty$ means $\psi = 0$.

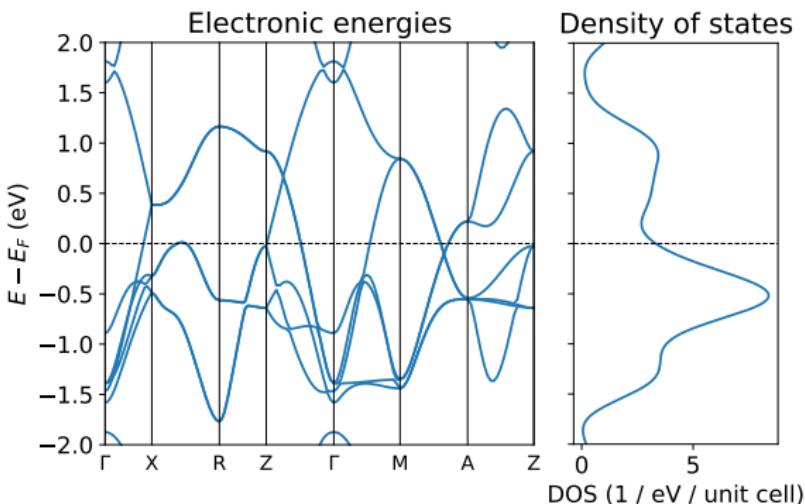
Crystal – a box with many particles?



- Periodic potential made by atoms.
- Multiple electrons per unit cell.

Electronic bands, density of states (DOS), Fermi level

- *Bands*: electronic energies for $\hat{H}\psi = E\psi$.
- *DOS*: histogram of the electronic energies.
- *Fermi level*: in the ground state, electronic energies filled up to Fermi level.



High Fermi level DOS can lead to superconductivity

- T_c depends strongly on Fermi level DOS.

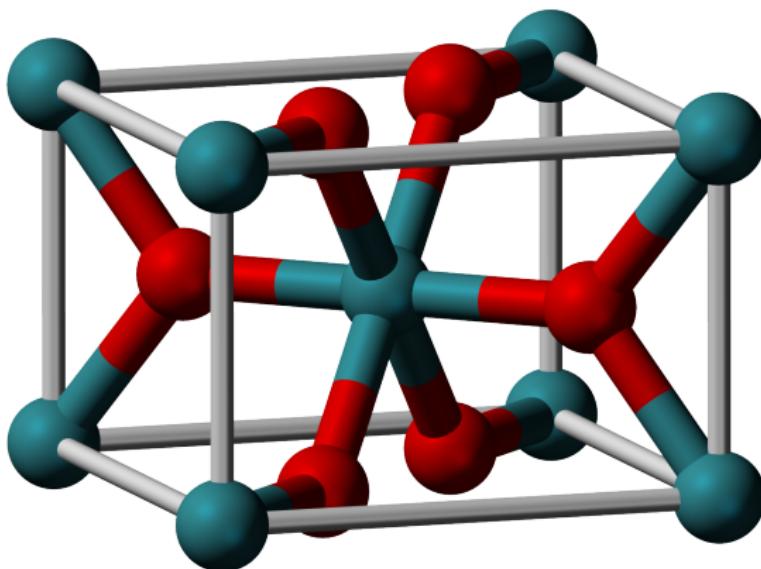
High Fermi level DOS can lead to superconductivity

- T_c depends strongly on Fermi level DOS.
- Strain shifts electronic energies, causing Fermi level DOS to change.
- Subsequent goal: *maximize Fermi level DOS*.

Strain and surrogate models

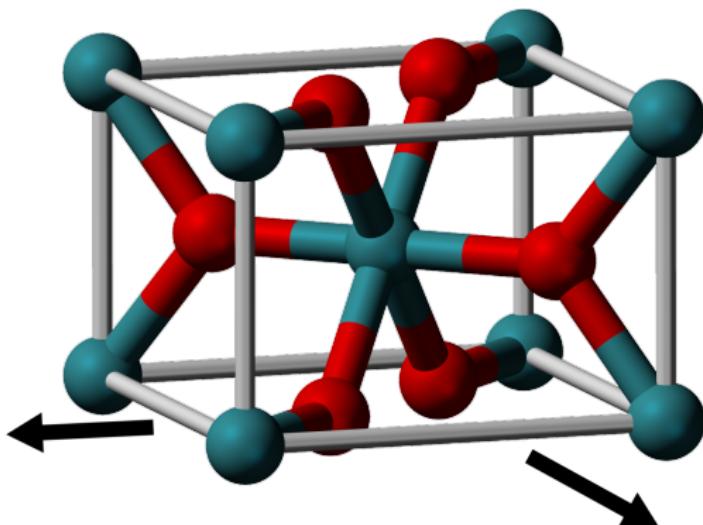
Strain: a deformation of the crystal

- A linear transformation applied to the crystal.
- Described by six numbers c_1, \dots, c_6 .



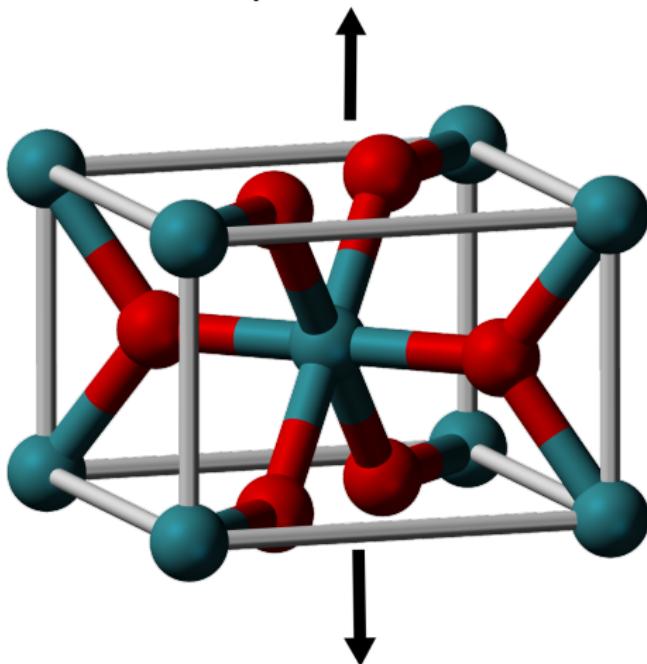
Positive c_1 strain: uniform expansion in the xy plane

- x and y coordinates multiplied by $1 + c_1$.
- z direction kept the same.



c_2 strain: expansion in the z direction

- z coordinate multiplied by $1 + \sqrt{2} c_2$.
- x and y directions kept the same.



Taylor-expanding electronic energies in the strain

- Strain is a small quantity ($\sim 5\%$).
- Taylor-expand electronic band energies to some finite order.

$$\epsilon_n(c_1, \dots, c_6; \mathbf{k}) \approx \epsilon_n(\mathbf{k}) + \sum_{i=1}^6 \frac{\partial \epsilon_n(\mathbf{k})}{\partial c_i} c_i$$

- Fit Taylor series coefficients to match DFT data.

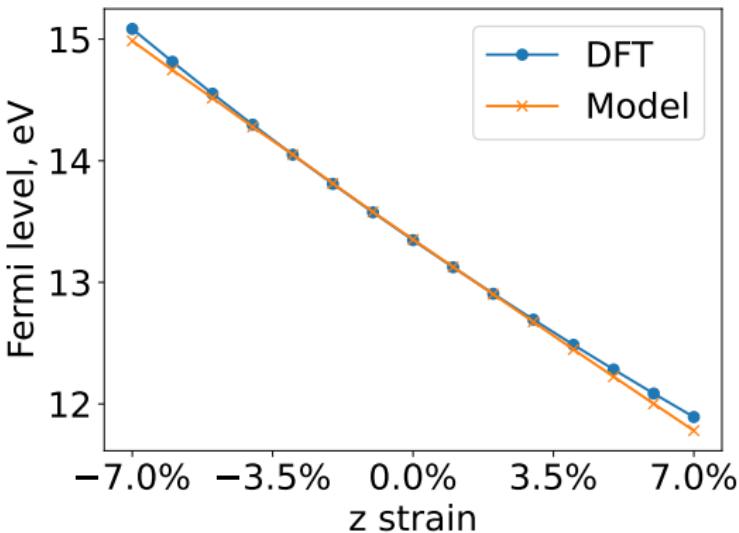
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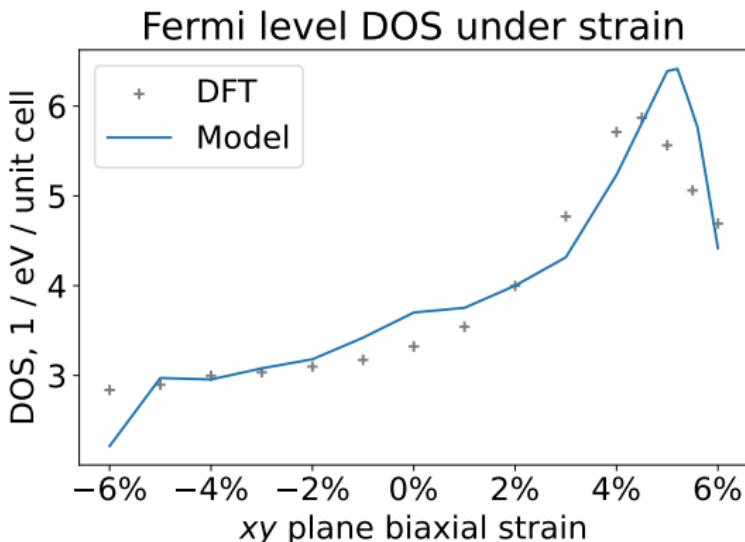
- Fit Taylor series coefficients to match DFT data.
- Predict DOS and Fermi level by counting electronic energies predicted by the bands model.

Performance of surrogate models



- Accurate even for very large strains.
- Almost instantaneous.

Performance of surrogate models



- Fermi level DOS: more nonlinearity, harder to predict.
- Decent accuracy.

Optimizing superconductivity

Maximizing Fermi level DOS by varying strain

- Model gives Fermi level DOS as a function of c_1, \dots, c_6 .
- Numerically search for best c_1, \dots, c_6 .
- Constraint: not allowed to strain by more than 5%.

Maximizing Fermi level DOS by varying strain

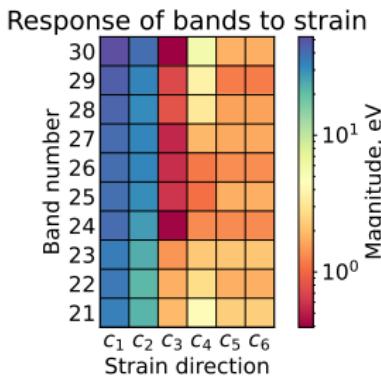
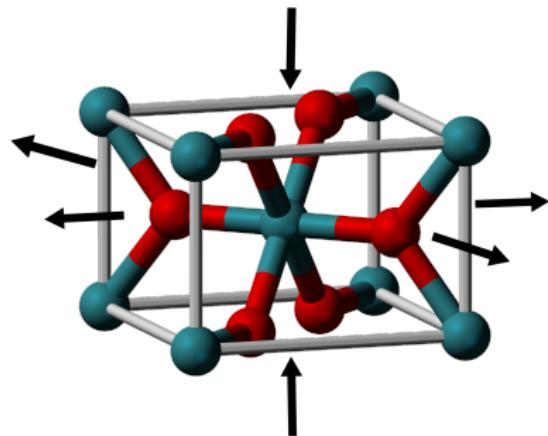
- Model gives Fermi level DOS as a function of c_1, \dots, c_6 .
- Numerically search for best c_1, \dots, c_6 .
- Constraint: not allowed to strain by more than 5%.
- Result: Fermi level DOS predicted to increase by 69% at strain

$$c_1 = 4.82\%, c_2 = -3.52\%, c_3 = -0.10\%, \\ c_4 = 0.05\%, c_5 = 0.24\%, c_6 = 0.25\%.$$

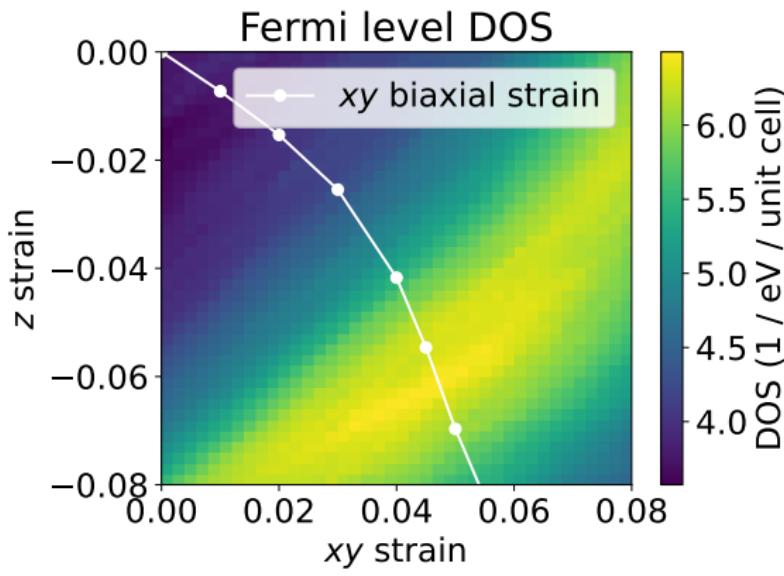
- Basically: large positive c_1 , large negative c_2 .

Optimal strain: expand in the xy plane, contract in the z direction

- c_1, c_2 strain have an outsized impact on the electronic bands – hence optimal strain almost entirely in c_1, c_2 .
- First known superconductivity-inducing strain, $\text{RuO}_2/\text{TiO}_2(110)$, is almost in the same direction.

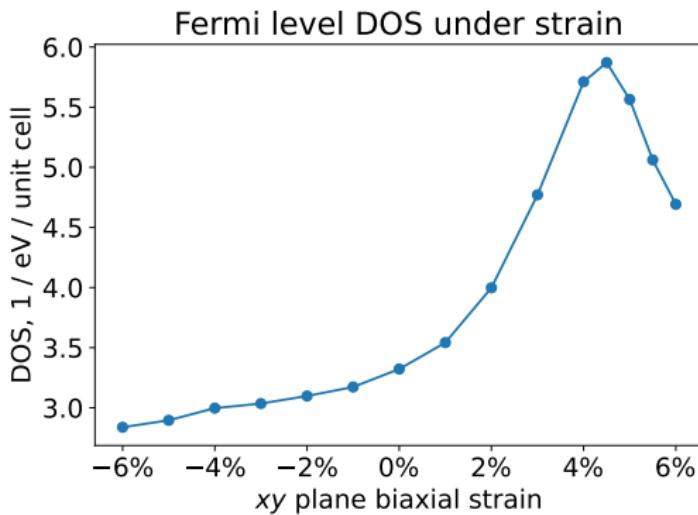


Optimal strain is very close to xy biaxial strain, which is experimentally accessible



- Stretch in the xy plane, let the z direction relax freely.
- Molecular Beam Epitaxy (MBE).

Fermi level DOS increase as predicted by DFT



- Predicted Fermi level DOS increase: 78%!
- For comparison, previous superconductivity-inducing strain brings on the order of 30%.

Prediction of superconductivity

- **Prediction:** if RuO_2 is subject to 4.5% tensile strain in the xy plane, superconductivity is likely to occur.
- Can potentially be realized in experiment using Molecular Beam Epitaxy (MBE) of RuO_2 in the (001) orientation.

Conclusion

Future work

- Possible superconductivity in RuO₂ under 4.5% tensile xy strain.
- Physical interpretation the coefficients of the electronic bands model.
- Apply modern ML techniques?
- Incorporate structural phase transitions into consideration.

Acknowledgements

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Bibliography

Appendix: molecular beam epitaxy

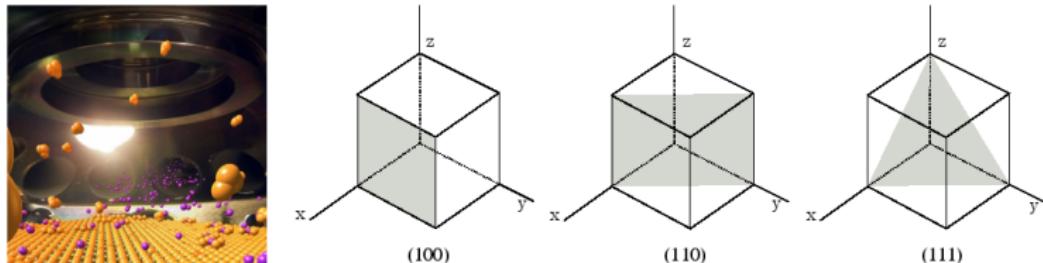


Figure: Epitaxy: molecules are sprinkled onto a substrate crystal prepared in some crystal orientation.

- Thin films resulting from epitaxy are strained.
- Discovery:² $\text{RuO}_2/\text{TiO}_2(110)$ thin films are superconducting.

²Ruf et. al. [ruf2021]

Appendix: deformation gradient, strain matrix

- Deformation gradient F : move point \mathbf{r} to $F\mathbf{r}$.
- Polar decomposition $F = UD$.
- Strain matrix $E = F - 1$. Symmetric 3×3 , so has 6 degrees of freedom.

$$E = c_1 \tau_1 + \cdots + c_6 \tau_6.$$

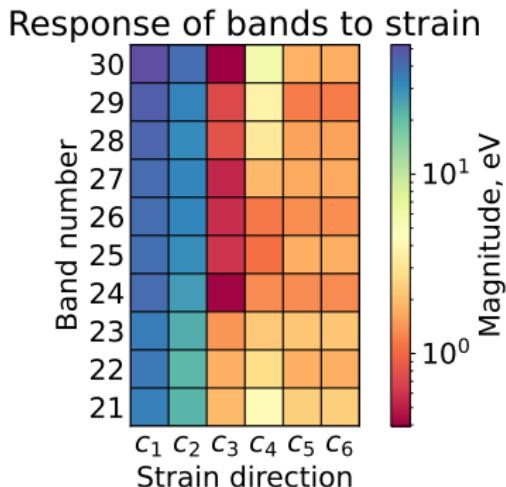
$$\begin{aligned}\tau_1 &= \begin{pmatrix} 1 & & \\ & 1 & \\ & & 0 \end{pmatrix}, & \tau_2 &= \begin{pmatrix} 0 & & \\ & 0 & \\ & & \sqrt{2} \end{pmatrix}, & \tau_3 &= \begin{pmatrix} 1 & & \\ & -1 & \\ & & 0 \end{pmatrix}, \\ \tau_4 &= \begin{pmatrix} 0 & 1 & \\ 1 & 0 & \\ & & 0 \end{pmatrix}, & \tau_5 &= \begin{pmatrix} 0 & & 1 \\ 0 & 0 & \\ 1 & & 0 \end{pmatrix}, & \tau_6 &= \begin{pmatrix} 0 & & \\ & 0 & 1 \\ & 1 & 0 \end{pmatrix}.\end{aligned}$$

Appendix: RuO₂/TiO₂(110) strain, the first strain known to induce superconductivity, is in a similar direction as the predicted optimal strain!

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

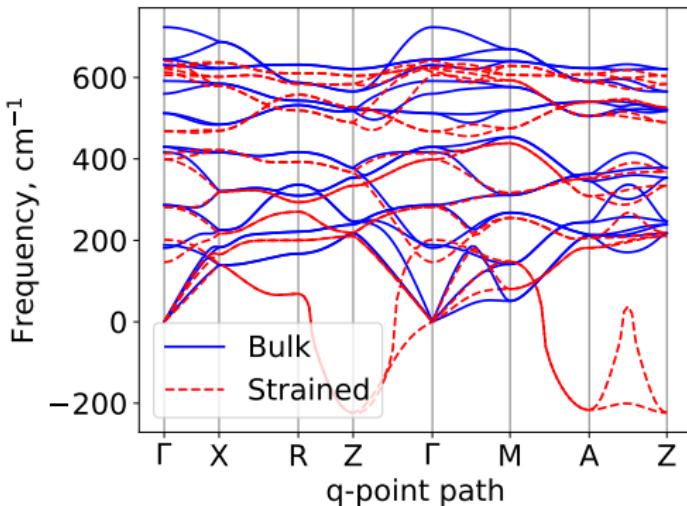
- RuO₂/TiO₂(110) strain: (2.2%, 2.3%, -4.7%).
- Optimized xy plane strain: (4.5%, 4.5%, -5.5%).
- Pretty closely aligned!

Appendix: high influence of c_1, c_2 on electronic bands causes the optimal strain to be almost exclusively comprised of c_1, c_2



- c_1 and c_2 strain directions have an outsized impact on the electronic energy bands

Appendix: possible softening of phonon modes



- Very preliminary possibility: softening of phonon modes.
- Need to do a careful convergence analysis of DFT results to gain more confidence.