

Large Language Models for Materials Discovery

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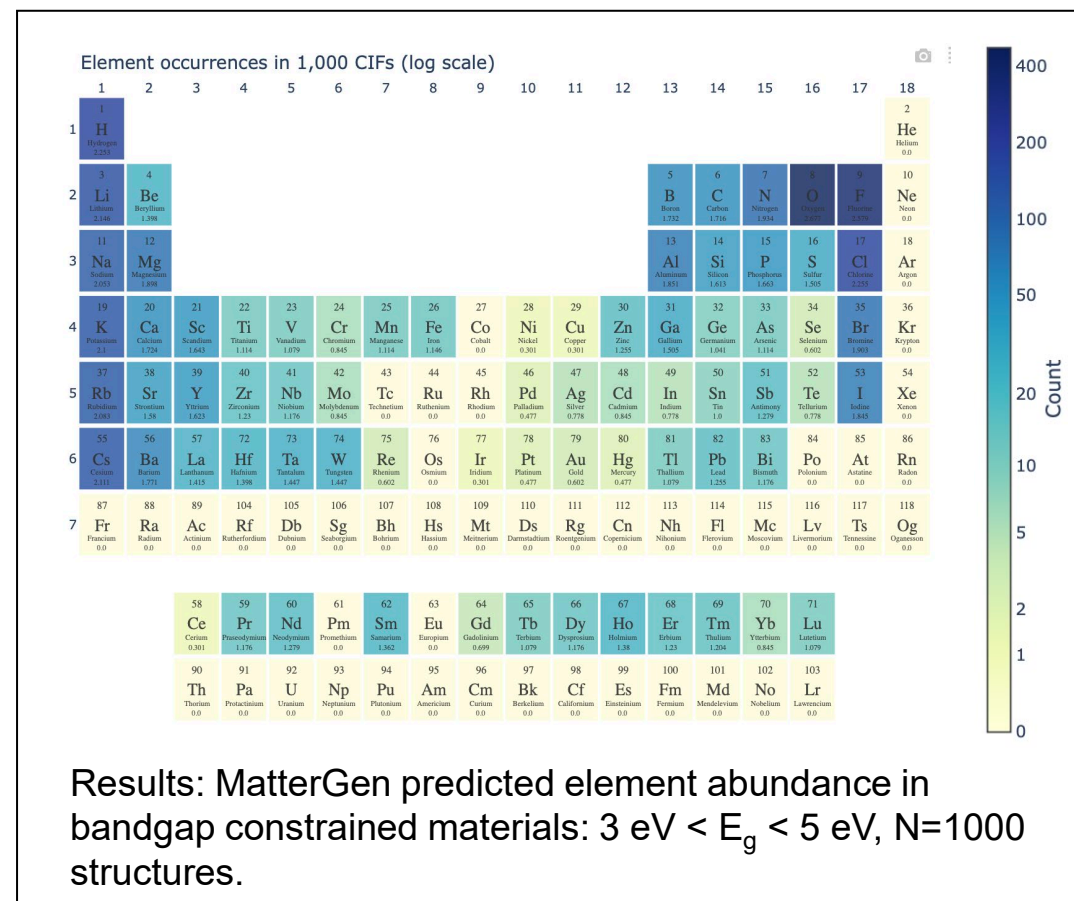
We used the Microsoft MatterGen framework and a pre-trained bandgap model to establish a workflow that utilizes ChatGPT style large language models for predicting new materials with constraint properties.

- Ported MatterGen successfully from GitHub to NMSU compute resource, Discovery.
- Tested implementation on Discovery, generated 1000 materials with constrained bandgap: $3 \text{ eV} < E_g < 5 \text{ eV}$, a range that is of interest for quantum sensing and quantum computing technologies.
- Timing information shows that it takes $\sim 18 \text{ s}$ to generate one material.

This result will enable us to expand research into two directions:

- Train models for custom properties.
- Better understand trade-offs between training set size and prediction error.

By undergraduate students
Daniel Reyes and Gavin Campos.



Transport Study of Small Polaron Trapping in TiO₂-based two-dimensional electron gases (2DEGs)

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The emergent superconductivity observed in RuO₂ thin films on TiO₂ substrates presents a puzzling question regarding its underlying mechanism. A striking parallel can be drawn with the case of monolayer FeSe on SrTiO₃, where strong interfacial electron-phonon coupling—particularly involving substrate phonons—was shown to play a crucial role in enhancing superconductivity. Motivated by this, we explored whether similar interfacial effects could be relevant in the RuO₂/TiO₂ system. To probe the electron-phonon properties from the TiO₂ substrate, we induced a two-dimensional electron gas (2DEG) at its surface through two methods: sputtering an amorphous SiO₂ (a-SiO₂) overlayer and ion milling. Both approaches introduce oxygen vacancies that dope electrons into the Ti 3d conduction band of TiO₂, forming a 2DEG. We have then patterned the 2DEG into Hall bars using photolithography. Transport measurements reveal that, unlike the metallic 2DEGs in STO or KTO, the TiO₂ 2DEG exhibits a metal-to-insulator crossover near 30 K. This insulating behavior at low temperature is attributed to small polaron trapping—a phenomenon closely related to electron-phonon coupling. Intriguingly, as the mobile carrier density approaches zero near the ground state, the Hall mobility remains finite, suggesting potential for low-carrier-density quantum devices such as quantum dots. Fitting the temperature dependence of the carrier density to Arrhenius behavior yields a small polaron trap energy of 4.4 meV. Our results shed light on the complex interplay between interfacial charge doping and polaron physics in TiO₂, providing a new perspective on the possible origins of superconductivity in RuO₂ heterostructures.

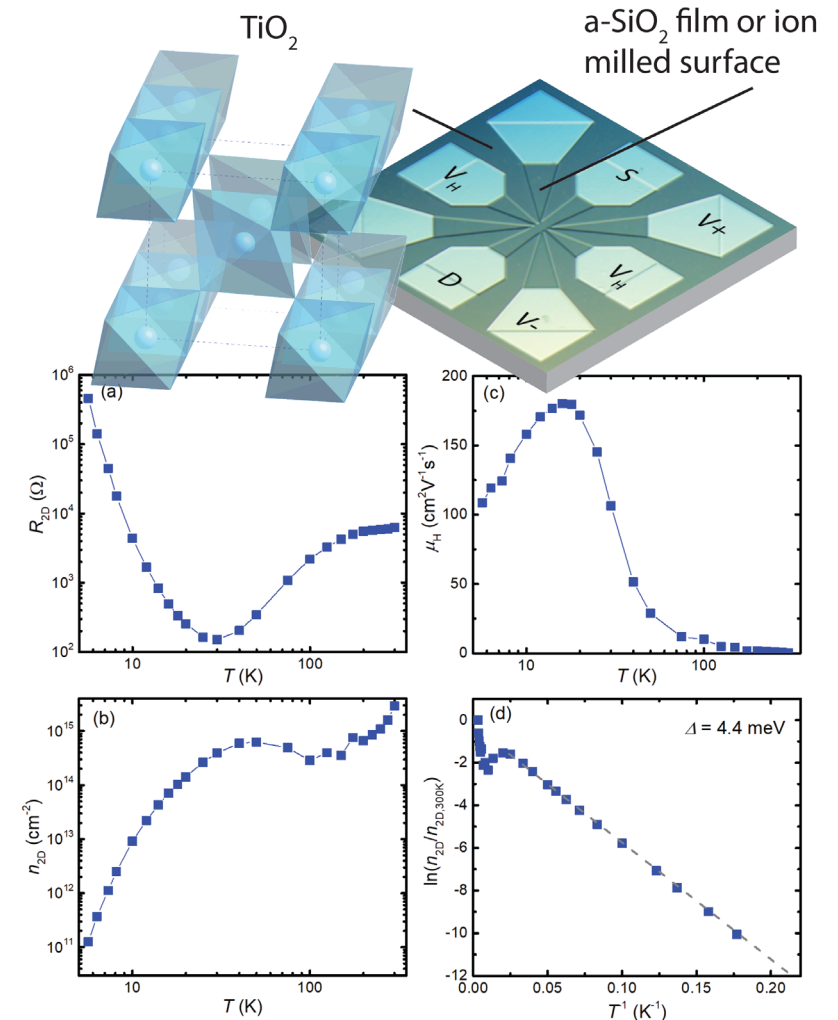


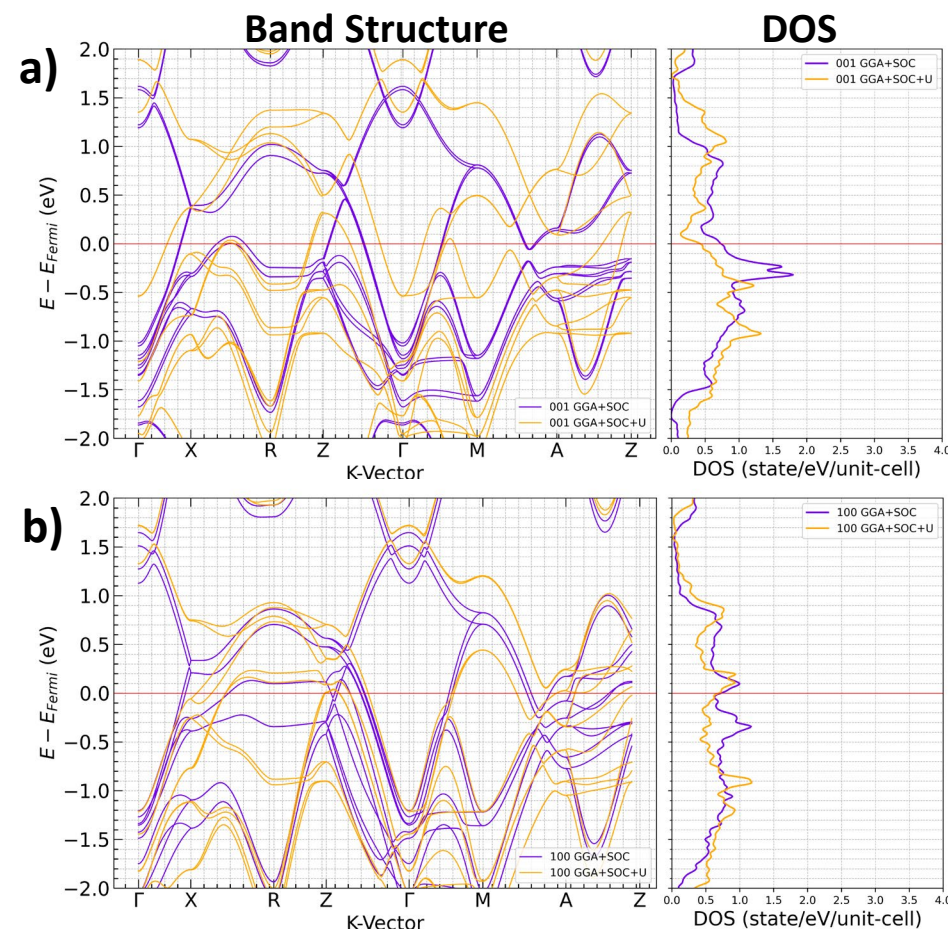
Image of of TiO₂-based 2DEGs device and transport characterization showing small polaron trapping.

Ab Initio Studies of the Electronic Structure and Electrical Transport in Epitaxially Strained RuO_2 Thin Films

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Gabriel Manzanares (MAP graduate student)

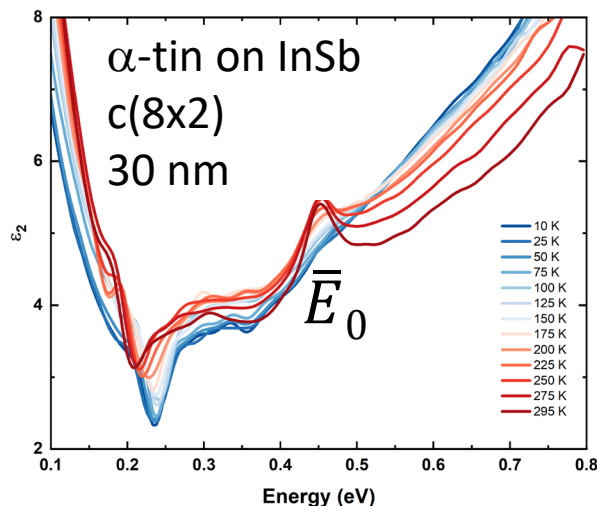
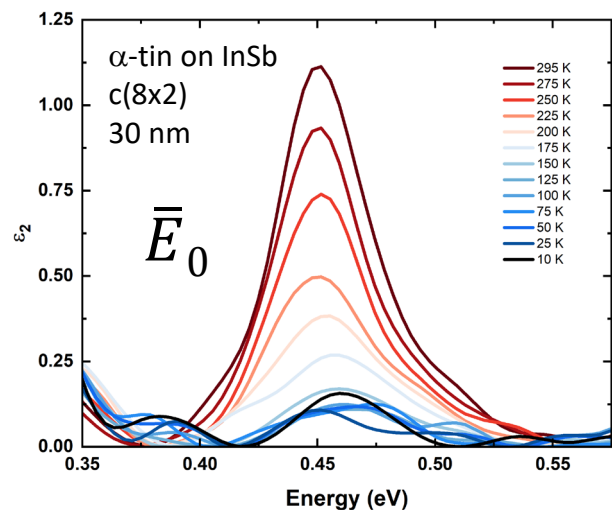
Recent discovery of strain-induced superconductivity in rutile RuO_2 thin films has attracted considerable attention. Superconducting behavior of RuO_2 films has been linked to the changes in the electronic structure of strained RuO_2 crystal lattice resulting in significant increase of the density of states at the Fermi level. Ab initio density functional computational methods were applied to study the influence of epitaxial strain and doping on the electronic and transport properties of RuO_2 thin films grown on TiO_2 substrates. The emergence of flat bands in the electronic structure of RuO_2 and their potential role in mediating superconductivity was investigated by applying biaxial epitaxial strain along the (001) and (100) crystal orientations of rutile RuO_2 . The results of this study suggest that the combined influence of strain and doping may offer a viable route to the stabilization of superconducting phases in RuO_2 thin films.



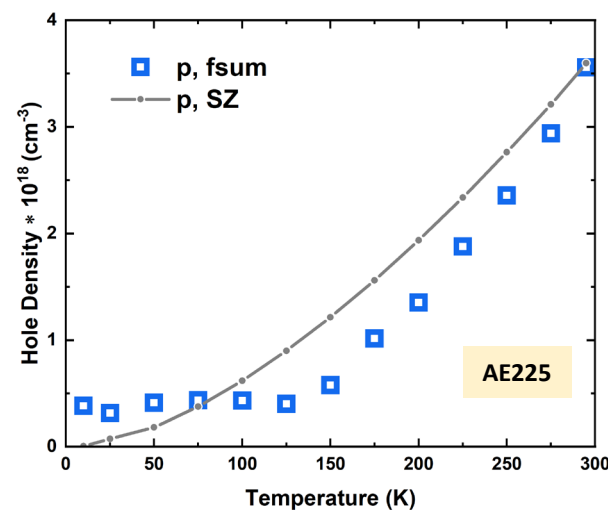
Calculated band structures and density of states of strained (a) (001) and (b) (100) RuO_2 thin films grown on TiO_2 substrate.

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 ϵ_2 from 300 K – 10 K $\bar{E}_0$ with linear background subtraction

Hole Density vs. Temperature

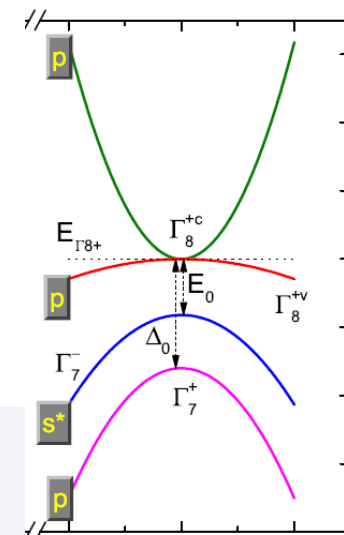


→ Ellipsometric angles modeled using basis spline functions for temperatures 300 K – 10 K to obtain the dielectric function for α-tin on InSb.

→ The f-sum rule is applied to the $\bar{E}_0$ absorption peak to determine the heavy hole density as a function of temperature.

$$\int_0^{\infty} \omega \epsilon_2(\omega) d\omega = \frac{\pi}{2} \omega_P^2$$

- f-sum rule: calculate carrier concentration from integrated absorption (oscillator strength).
- Direct gap absorption for 30 nm α-Sn on InSb (100) c(8x2) constant up to 150 K due to transitions into the light “hole” conduction band.
- Direct gap absorption increases above 150 K due to thermal excitation of heavy holes.
- Good agreement with theory for heavy hole mass $m_{hh}=0.26$. (Zollner, JVSTB, 2025.)



α-tin on InSb grown by A. Engel and C. Palmstrom