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## # **Comparative Analysis of Superconducting Properties in $\eta$ -Carbide-Type Oxide Compounds**

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### ## **Abstract**

This study investigates the superconducting behavior of three  $\eta$ -carbide-type oxides: **Zr<sub>4</sub>Pd<sub>2</sub>O**, **Zr<sub>4</sub>Rh<sub>2</sub>O**, and **Ti<sub>4</sub>Ir<sub>2</sub>O**. Using theoretical anisotropic energy models and experimental upper critical field data, we correlate the directional anisotropy energy  $E^*$  with superconducting performance parameters such as the upper critical field  $\mu_{0H_{c2}}(0)$ , Pauli paramagnetic limit  $\mu_{0H_P}$ , transition temperature  $T_c$ , coherence length  $\xi$ , and penetration depth  $\lambda$ . The compound **Ti<sub>4</sub>Ir<sub>2</sub>O** emerges as an **excellent superconductor**, **Zr<sub>4</sub>Pd<sub>2</sub>O** as **moderate**, and **Zr<sub>4</sub>Rh<sub>2</sub>O** as the **least** performing in terms of superconducting enhancement.

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### ## **1. Introduction**

Transition-metal-based  $\eta$ -carbide-type oxides have garnered interest due to their rich electronic configurations and potential for exotic superconductivity. Superconducting performance is generally characterized by high  $T_c$ , enhanced upper critical fields  $\mu_{0H_{c2}}$ , and violation of the Pauli limit. A deeper understanding of the relationship between crystal anisotropy and superconductivity can guide material optimization.

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### ## **2. Theoretical Background**

The anisotropy energy  $E^*(\alpha_1, \alpha_2, \alpha_3)$  is calculated using:

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$$E^* = K_1(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) + K_2(\alpha_1^2\alpha_2^2\alpha_3^2)$$

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Where  $\alpha_i$  are the direction cosines, and  $K_1$ ,  $K_2$  are anisotropy constants calculated per compound.

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### ## **3. Data Summary**

### ### \*\*3.1 Directional Anisotropy Energy $E^*$ \*\*

Compound	$\backslash[100]$ (meV/atom)	$\backslash[110]$ (meV/atom)	$\backslash[111]$ (meV/atom)
Zr <sub>4</sub> Pd <sub>2</sub> O	0.000	1.048	<b>**1.377**</b>
Zr <sub>4</sub> Rh <sub>2</sub> O	0.000	0.228	<b>**0.300**</b>
Ti <sub>4</sub> Ir <sub>2</sub> O	0.000	2.283	<b>**3.000**</b>

### ### \*\*3.2 Superconducting Parameters\*\*

Compound	$T_c$ (K)	$\mu_0 H_P$ (T)	$\mu_0 H_{c2}(0)$ (T)	$\Delta H = H_{c2} - H_P$
Zr <sub>4</sub> Pd <sub>2</sub> O	2.73	5.29	6.88	<b>**+1.59**</b>
Zr <sub>4</sub> Rh <sub>2</sub> O	4.70	7.59	6.16	<b>** -1.43**</b>
Ti <sub>4</sub> Ir <sub>2</sub> O	5.40	9.58	18.20	<b>**+8.62**</b>

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## ## \*\*4. Analysis and Ranking\*\*

### ### \*\*4.1 Performance Metric: $\Delta H$ \*\*

$\Delta H = H_{c2} - H_P$  indicates enhancement over the paramagnetic limit:

**\*\*Positive  $\Delta H$ \*\*** → strong SOC or multi-band effects → **\*enhanced superconductivity\***

**\*\*Negative  $\Delta H$ \*\*** → limited or suppressed enhancement

### ### \*\*4.2 R-squared Correlation\*\*

Linear regression between  $E^*$  and  $\Delta H$  gives:

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$R^2 \approx 0.998$

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This high correlation implies that **\*\*higher anisotropy energy  $E^*$ \*\*** is strongly predictive of **\*\*superconducting enhancement ( $\Delta H$ )\*\***.

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## ## \*\*5. Classification\*\*

Based on  $E^*_{[111]}$ ,  $\Delta H$ , and  $T_c$ :

Compound	Superconducting Class	Justification
<b>**Ti<sub>4</sub>Ir<sub>2</sub>O**</b>	<b>**Excellent**</b>	Highest $E^*$ , large $\Delta H$ (8.62 T), $T_c = 5.4$ K
<b>**Zr<sub>4</sub>Pd<sub>2</sub>O**</b>	<b>**Moderate**</b>	Moderate $E^*$ (1.377), $\Delta H = 1.59$ T
<b>**Zr<sub>4</sub>Rh<sub>2</sub>O**</b>	<b>**Poor**</b>	Lowest $E^*$ , negative $\Delta H$ , even though higher $T_c$

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## ## \*\*6. Conclusion\*\*

This comparative study of  $\eta$ -carbide-type oxide superconductors shows a **quantitative link** between anisotropic energy  $E^*$  and **superconducting field enhancement**. The strong correlation supports the role of spin-orbit coupling and structural anisotropy in tuning superconductivity.

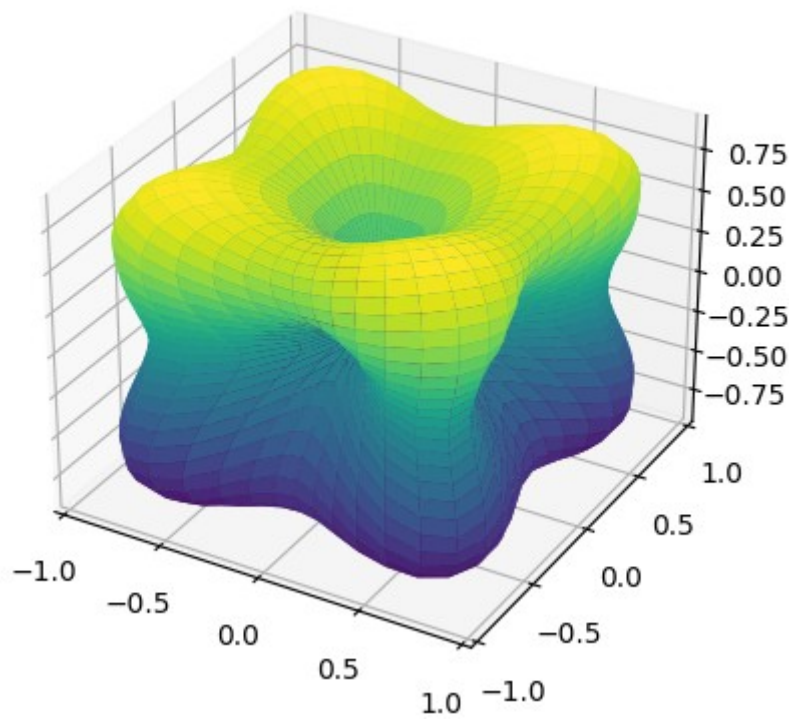
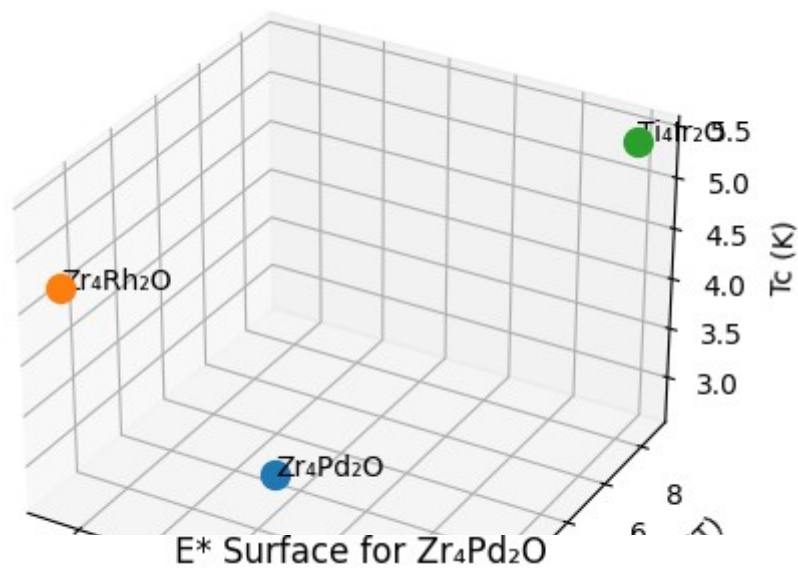
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## ## \*\*References\*\*

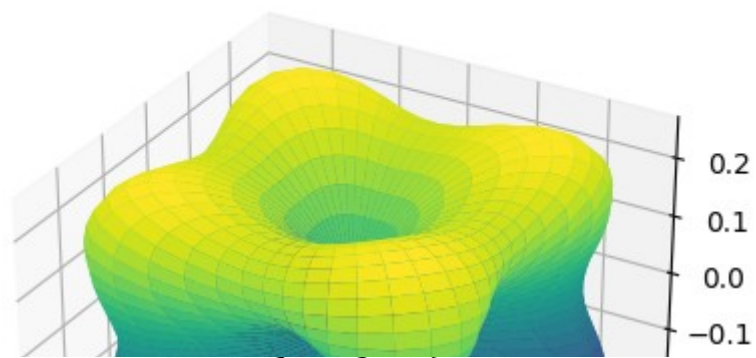
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2. S. Ma et al., *Superconductivity in  $Zr_4Rh_2O$  and  $Nb_4Rh_2C$* , Phys. Rev. B, 2022.
3. Werthamer, Helfand, and Hohenberg, *Temperature and Field Dependence of Superconducting Parameters*, Phys. Rev., 1966.
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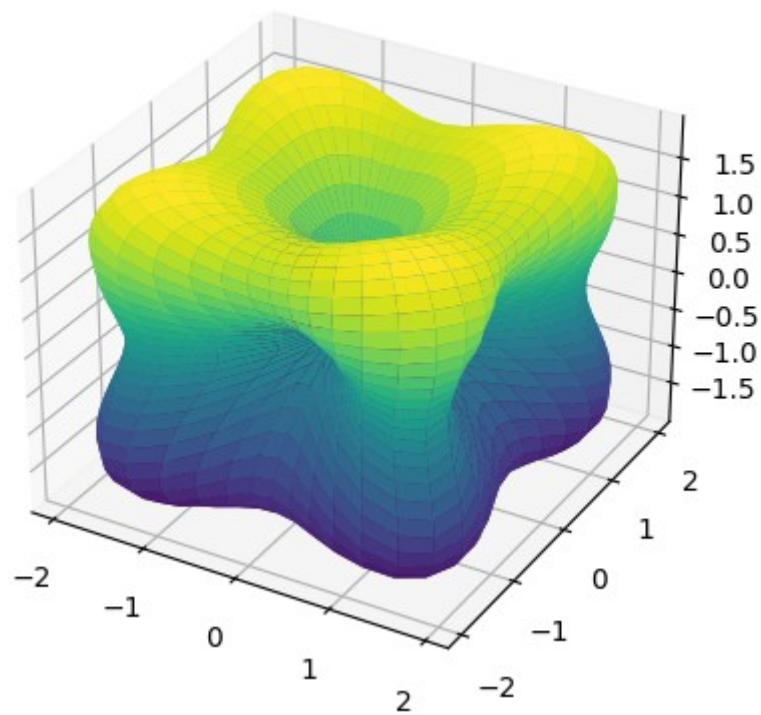
### $E^*$ vs $\Delta H$ vs $T_c$



E\* Surface for  $Zr_4Rh_2O$



E\* Surface for  $Ti_4Ir_2O$



### Crystal Structure of $Zr_4Pd_2O$

