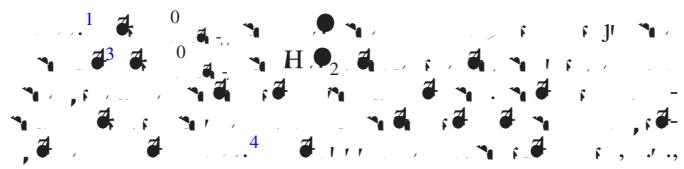


**Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides:
Magnetically interacting cation vacancies and theeT_{0.4857006.4857415.2396577.2104}Tm_{0.7}T_{0.2}**



H_2 molecule at 10^8

II. METHODS

A. Calculation of the magnetic configuration of a single vacancy

21
520
96
 $2 \times 2 \times 2$ k-
 Γ - 4 \times 4 \times 4 k-
7429 0 -3k j/22 -304 5 17.913.023.3382.6517 -35 0 -3k 0 + 0 -3k

C. Calculation of the magnetic interaction range

$$E_{\frac{M}{N}}(x) = \frac{1}{N} \sum_{i=1}^N H_i(x) + \Delta E_{\frac{M}{N}}(x) = E_{\frac{M}{N}}(x)$$

$$\Delta E_{\frac{M}{N}}(x) = \left(\frac{M}{N} \right) \sum_{i=1}^N \left(\frac{H_i(x)}{M} - \frac{1}{N} \right)^2$$

D. Calculation of the percolation staircase

$$E_{\frac{M}{N}}(x) = \frac{1}{N} \sum_{i=1}^N H_i(x) + \Delta E_{\frac{M}{N}}(x)$$

$$\Delta E_{\frac{M}{N}}(x) = \lambda \sum_{i=1}^N \left(\frac{H_i(x)}{\lambda} - \frac{1}{N} \right)^2$$

$$\lambda = \left(\frac{M}{N} \right) x = [\]/N, \quad i \in N$$

$$H_i(x) = \sum_{j=1}^N x_{i,j} \delta_{i,j}$$

$$x_{i,j} = x_{i,j}(\lambda, x) = \frac{1}{N} \sum_{k=1}^N \delta_{i,k} \delta_{j,k}$$

$$\delta_{i,j} = \frac{1}{M} \sum_{m=1}^M \delta_{i,m} \delta_{j,m}$$

$= 1$

1() 1(),
1()
1()

**B. Results for the formation enthalpies and transition energies
of Hf and O vacancies and equilibrium concentration of
magnetic defects in HfO_2**

3
H
 HfO_2
H

D. Results for the percolation threshold for the cation sublattice of the HfO₂ Baddeleyite structure

Figure 5 shows the results for the percolation threshold for the cation sublattice of the HfO₂ Baddeleyite structure. The figure consists of two panels. The left panel shows the fraction of Hf⁴⁺ ions in the A sites (x_{Hf}^A) versus the volume fraction of Hf⁴⁺ ions in the lattice (x). The right panel shows the fraction of Hf⁴⁺ ions in the B sites (x_{Hf}^B) versus x . Both panels show a sharp increase in the fraction of Hf⁴⁺ ions at a certain value of x , which corresponds to the percolation threshold. The percolation threshold for the A-site cation sublattice is approximately $x = 30.5\%$, and for the B-site cation sublattice is approximately $x = 13.5\%$.

C. Results for the range of V_{Hf}V_{Hf}²⁺ magnetic interactions in HfO₂

The energy difference between the ground state and the excited state of the V_{Hf}V_{Hf}²⁺ magnetic interaction in HfO₂ is given by:

$$\Delta E(\omega) = E(\omega) - E(0) \approx 205 \text{ meV}$$

where ω is the frequency of the magnetic interaction. The energy difference is proportional to the square of the frequency, so we can write:

$$\Delta E(\omega) = \frac{1}{2} \mu_B^2 \omega^2$$

where μ_B is the Bohr magneton. The value of μ_B is approximately $1 \mu_B$. Substituting this value into the equation, we get:

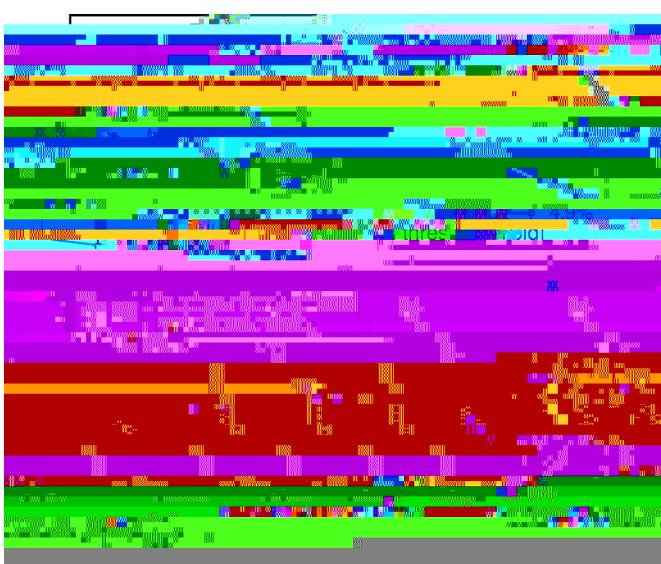
$$\Delta E(\omega) = 74 \text{ meV}$$

for $\omega = 2.6 \times 10^8 \text{ Hz}$. The energy difference is also proportional to the concentration of Hf⁴⁺ ions, so we can write:

$$\Delta E(\omega) = 8 \text{ meV}$$

for $x = 6.4 \times 10^{-3}$. This result is consistent with the experimental observation that the magnetic interaction between Hf⁴⁺ ions in HfO₂ is very weak.

IV. CONCLUSION

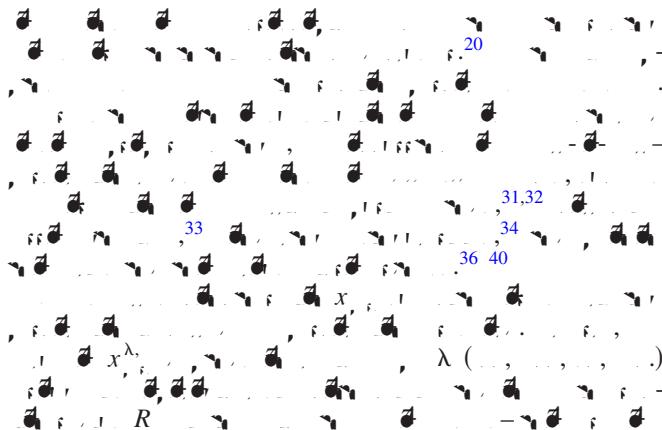
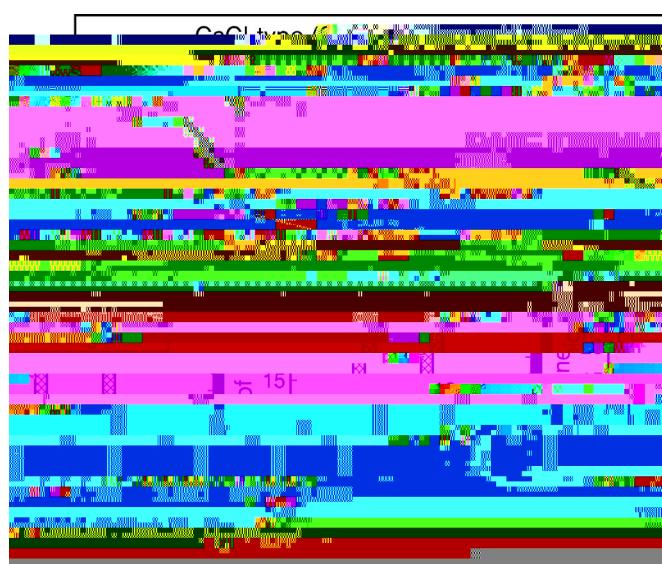


APPENDIX: PERCOLATION STAIRCASES IN COMMON LATTICES



The figure consists of a series of horizontal bands of varying colors and patterns. From top to bottom, the colors transition through blue, green, yellow, red, purple, orange, pink, light blue, and finally a darker red at the bottom. Each band contains numerous small, distinct elements such as dots, squares, and lines in various colors like black, white, yellow, red, green, blue, and purple. Some bands have a more uniform pattern, while others show more complex, overlapping structures. The overall effect is a dense, abstract representation of data or a sequence of frames.

A musical score for piano, page 7, featuring ten measures of music. The score includes two staves: a treble clef staff and a bass clef staff. The music consists of eighth and sixteenth note patterns, with some notes having stems pointing up and others down. Measure 10 concludes with a double bar line and repeat dots, indicating a section to be repeated.



A horizontal row of 12 small square boxes, each containing a different Indian musical note (shabda).

34
 R
 λ
 x^λ
 (\dots)
 $= \dots = x^\lambda$
 (\dots, ϵ, \dots)
 M
 M
 M
 λ
 $(\dots) x$
 $45 R$
 20
 R
 λ
 33
 $6,41,42$
 x^λ
 M
 x^λ
 R
 $= R_1, R_2 R$

Let $\lambda = \lambda_1 \cup \dots \cup \lambda_k$ be a partition of N ($\lambda_i \in \{1, \dots, N\} \subset \{1, \dots, N\}$). Then λ is called a partition of N into k parts.

11.