Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides: Magnetically interacting cation vacancies and theeTf6.4857006.4857415.2396577.2104Tm(2)T

[illegible] H [illegible] $_2$ [illegible] H [illegible] 10^8.

II. METHODS

A. Calculation of the magnetic configuration of a single vacancy

[illegible] ([illegible] - [illegible]) [illegible].[21] [illegible] 520 [illegible] 96 [illegible] $2\times2\times2$ **k**- [illegible] Γ- [illegible] $4\times4\times4$ **k**- [illegible] 7429 [illegible], 0 [illegible] 3k [illegible]/ 22 [illegible] -304 [illegible] 5 [illegible] 17.913.023.3382.6517 -35 0 [illegible] 3k [illegible] + 0 [illegible] 3k

C. Calculation of the magnetic interaction range

[illegible] $\Delta E(\;) = E(\;)$ [illegible] $E(\;)$ [illegible] $^{0}_{\mathrm{H}}$ [illegible]

D. Calculation of the percolation staircase

[illegible] λ [illegible] $x = [\;]/N,$ [illegible] N [illegible] $x(\lambda,\;)$ [illegible] $x(\lambda,\;)$ [illegible]

[illegible] $= 1$

[illegible]

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

[illegible]

[illegible] ($_{\mathrm{H}}$). [illegible] (T [illegible] < 2000 K) [illegible] $^{2+}$ (T [illegible] > 2000 K).

C. Results for the range of V_{Hf}-V_{Hf} magnetic interactions in HfO$_2$

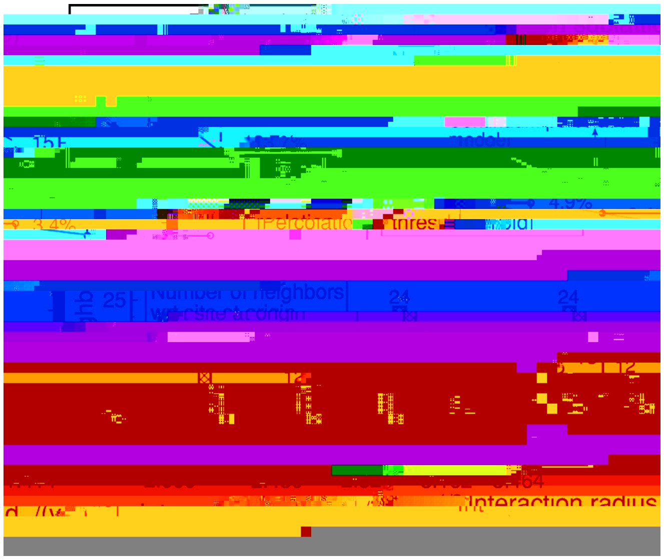
[illegible] ΔE [illegible] $=E$ [illegible] E [illegible] $^0_{\mathrm{H}}$ [illegible] 96- [illegible] 205 [illegible] 39 [illegible] ($\mu = 1\mu_B$) [illegible] ΔE [illegible] $=$ 74 [illegible] $=2.6$ [illegible] ΔE [illegible] $=$ 8 [illegible] $=6.4$ [illegible].

D. Results for the percolation threshold for the cation sublattice of the HfO$_2$ Baddelayite structure

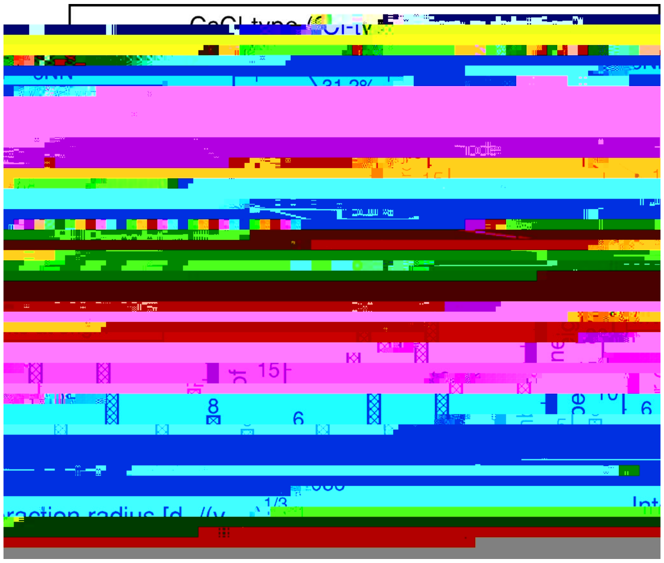
[illegible] 5 [illegible] H [illegible]$_2$. [illegible] [illegible]$_2$). [illegible] 16 [illegible] 6 [illegible] 0.25 [illegible] H [illegible] H [illegible]$_2$ [illegible] $=$ [illegible] $_1$ [illegible] $x = 30.5\%$. [illegible] H [illegible] $x = 13.5\%$ [illegible] H [illegible]$_2$ [illegible] H [illegible] H [illegible]$_2$ [illegible] 10^8.

IV. CONCLUSION

[illegible] H [illegible]$_2$ [illegible]: () [illegible] ()



6. [illegible]



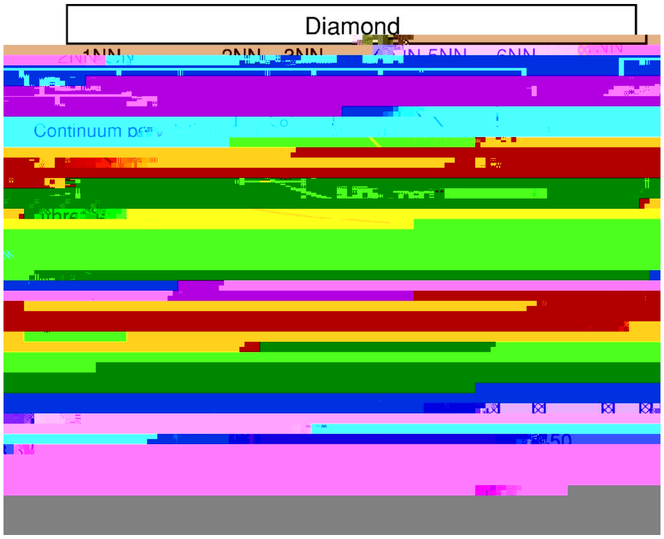
8. [illegible]

APPENDIX: PERCOLATION STAIRCASES IN COMMON LATTICES

[illegible] [31,32] [illegible] [33] [illegible] [34] [illegible] [35] [illegible]

[illegible] [20] [illegible] [31,32] [illegible] [33] [illegible] [34] [illegible] [36–40] [illegible]

7. [illegible]



9. [illegible]

[34]

R (

), R

H

5 15 [6,41,42]

$x^{\lambda,}$

(, ,) λ

= = [43,44]

x :

(, ϵ , ,) M

M

M

λ

( ) x

[45] R

[20] (

R J)

[33] R

[6,41,42] λ,

$x^{\lambda,}$

M $x^{\lambda,}$ R

$=R_1$ $,R_2$ R

$\lambda=\lambda \cup \cdots \cup \lambda$ ($\{\,,\ldots,\,\}\subset\{1,\ldots,N\}$). x λ, λ λ 11.

---

[1] k, k, **89**, 216403 (2002).

[2] k, ( ) **430**, 630 (2004).

[3] **94**, 217205 (2005).

[4] k, **4**, 173 (2005).

[5] k, **72**, 024450 (2005).

[6] **96**, 107203 (2006).

[7] **96**, 207602 (2006).

[8] H. **73**, 132410 (2006).

[9] k, **90**, 026801 (2003).

[10] **72**, 658 (2005).

[11] *C B M* (, , 2006), . 483.

[12] H. H , k, **73**, 132404 (2006).

[13] **74**, 161306( ) (2006).

[14] k, *R D S* (, , 1964).

[15] *T y D S* (, , 1975).

[16] **16**, 1209 (1975).

[17] H **7**