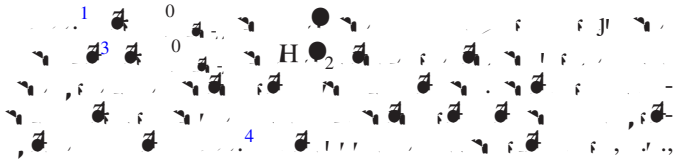
Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides: Magnetically interacting cation vacancies and theeT6.4857006.4857415.2396577.2104Tm(?)T



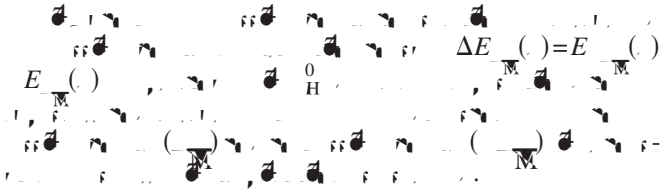
H 2 - H 10^8.

II. METHODS

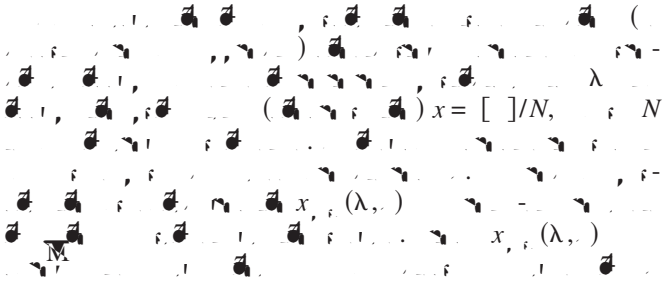
A. Calculation of the magnetic configuration of a single vacancy

(-) [21] 520 . 96 2×2×2 k- Γ- 4×4×4 k- 7429 , 0 3k J/ 22 -304 5 17.913.023.3382.6517 -35 0 3k + 0 3k

C. Calculation of the magnetic interaction range



D. Calculation of the percolation staircase



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).
(T,
<2000 K)
2+ (T,
>2000 K).

C. Results for the range of V_{Hf}-V_{Hf} magnetic interactions in HfO_2

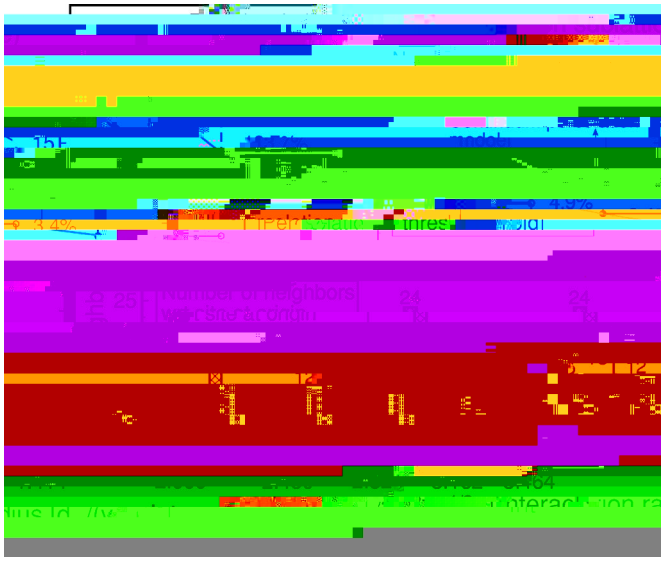
ΔE ( )=E ( ) E ( ) 0 H
96-
205
(,)
39
(μ=1μ_B)
, ., ΔE ( )= 74
=2.6 ( ),
ΔE ( )= 8
=6.4 .

D. Results for the percolation threshold for the cation sublattice of the HfO_2 Baddelayite structure

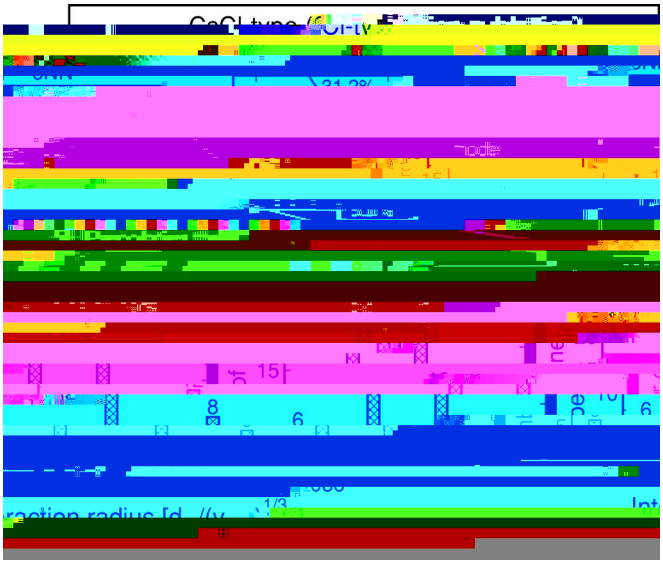
5
H 2.
(., , 2).
16 6
, –; . .,
0.25 .
H
H 2 = 1 x=30.5%.
H
x=13.5%
H 2 H
H 2
10^8.

IV. CONCLUSION

H 2
: ( )
( )



. 6. ( ) ( ) k ( ) .



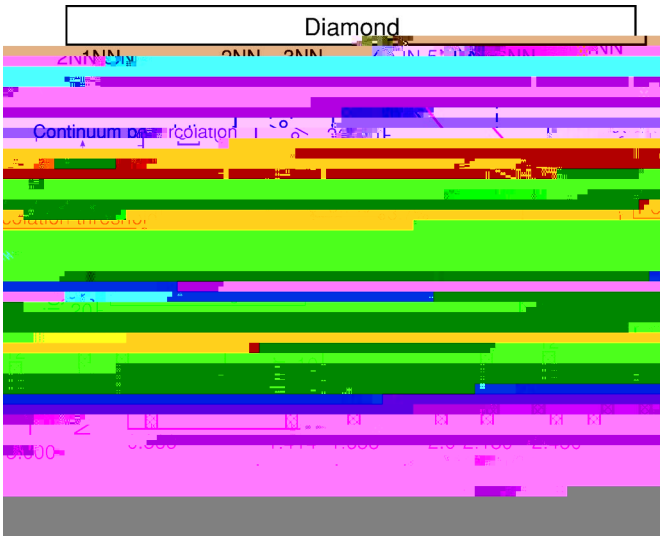
. 8. ( ) ( ) ( ) .

APPENDIX: PERCOLATION STAIRCASES IN COMMON LATTICES

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

. 7. ( ) ( ) 2 3 ( ) .

[20] [31,32] [33] [34] [36 40] x, x^{λ}, λ (, , , .) R –



. 9. ( ) ( ) ( ) .

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

[1] … **89**, 216403 (2002).
[2] … **430**, 630 (2004).
[3] … **94**, 217205 (2005).
[4] … **4**, 173 (2005).
[5] … **72**, 024450 (2005).
[6] … **96**, 107203 (2006).
[7] … **96**, 207602 (2006).
[8] H. … **73**, 132410 (2006).
[9] … **90**, 026801 (2003).
[10] … **72**, 658 (2005).
[11] … *C* … *B* … *M* … 2006), … 483.
[12] … H. H … **73**, 132404 (2006).
[13] … **74**, 161306( ) (2006).
[14] … *R* … *D* … *S* … 1964).
[15] … *T* … *y* … *D* … *S* … 1975).
[16] … **16**, 1209 (1975).
[17] … H … **7**