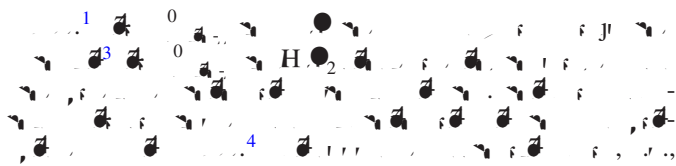


**Nonstoichiometry as a source of magnetism in otherwise nonmagnetic oxides:**

**Magnetically interacting cation vacancies and the  $T_{\text{M}}$**



$H_{21} = 10^8$

## II. METHODS

### A. Calculation of the magnetic configuration of a single vacancy

The calculation of the magnetic configuration of a single vacancy is performed using the following parameters:

- Number of sites: 520
- Number of spins: 96
- Exchange interaction:  $2 \times 2 \times 2$  k
- Crystal field splitting:  $\Gamma = 4 \times 4 \times 4$  k
- Energy values: 7429, 0, 3k, j/22, -304, 5, 17.913.023.3382.6517 -35, 0, 3k, r + 0, 3k

### C. Calculation of the magnetic interaction range

$$\Delta E_{\mathbf{M}}(\mathbf{r}) = E_{\mathbf{M}}(\mathbf{r}) - E_{\mathbf{M}}(\mathbf{0})$$

### D. Calculation of the percolation staircase

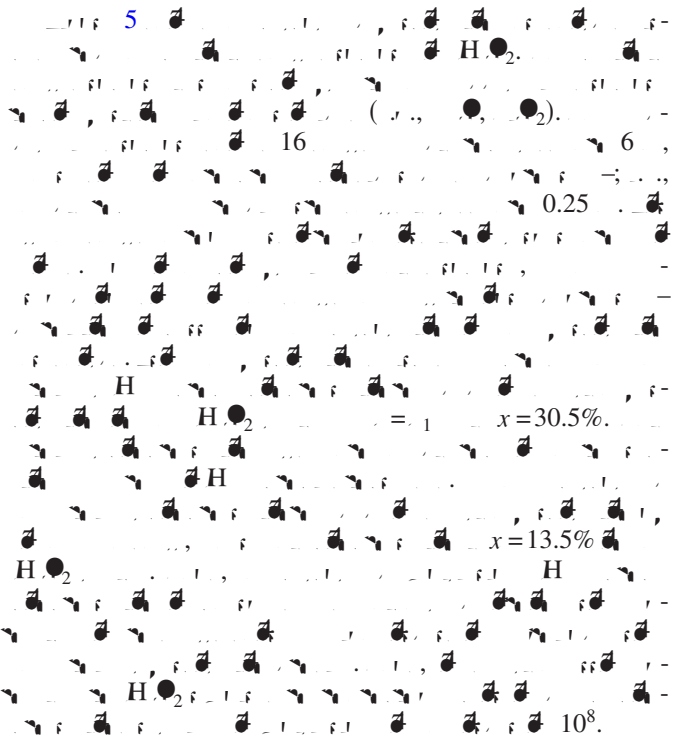
$$x_{\mathbf{M}}(\lambda, \mathbf{r}) = \left[ \frac{\lambda}{N} \right]$$

1( ) 1( ),  $\dots$

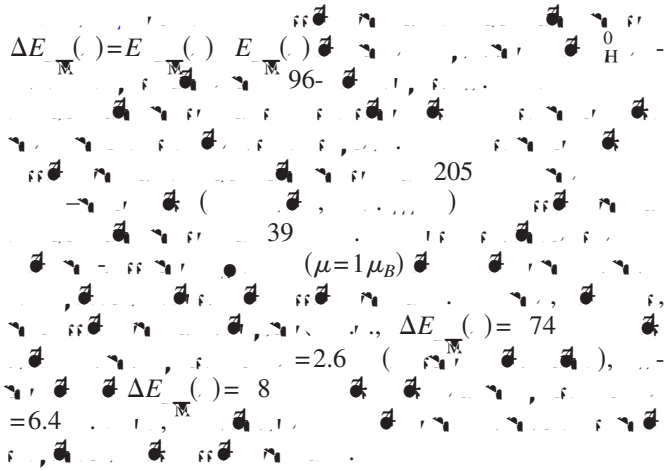
**B. Results for the formation enthalpies and transition energies of Hf and O vacancies and equilibrium concentration of magnetic defects in HfO<sub>2</sub>**

3  $\dots$

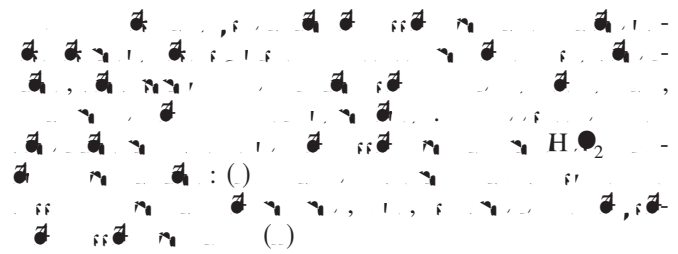
**D. Results for the percolation threshold for the cation sublattice of the HfO<sub>2</sub> Baddelayite structure**



**C. Results for the range of  $V_{Hf}-V_{Hf}$  magnetic interactions in HfO<sub>2</sub>**



**IV. CONCLUSION**



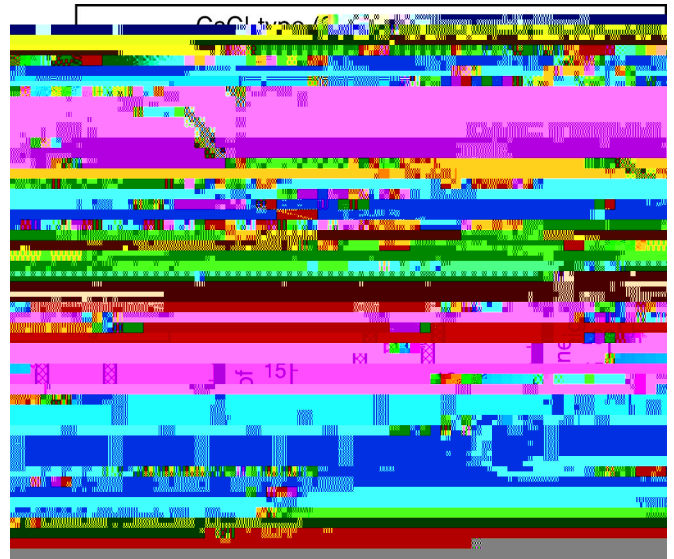
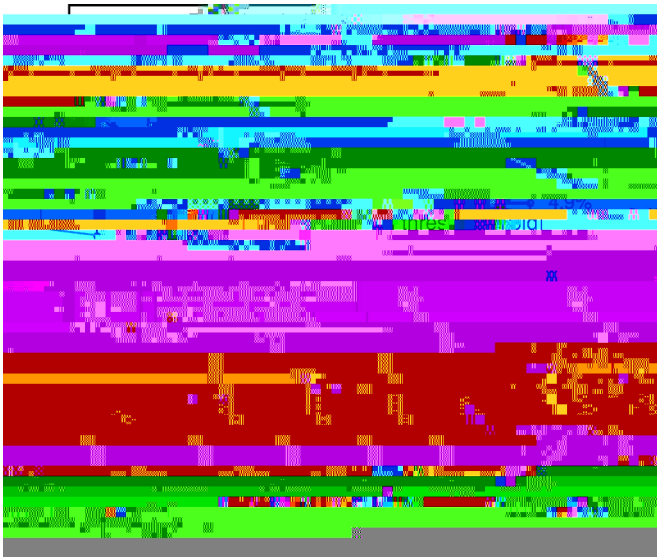


FIG. 6. (Color online) Percolation staircase on a lattice. The colors represent different clusters. The horizontal axis is the site index  $i$  and the vertical axis is the site index  $j$ .

FIG. 8. (Color online) Percolation staircase on a lattice. The colors represent different clusters. The horizontal axis is the site index  $i$  and the vertical axis is the site index  $j$ .

**APPENDIX: PERCOLATION STAIRCASES IN COMMON LATTICES**

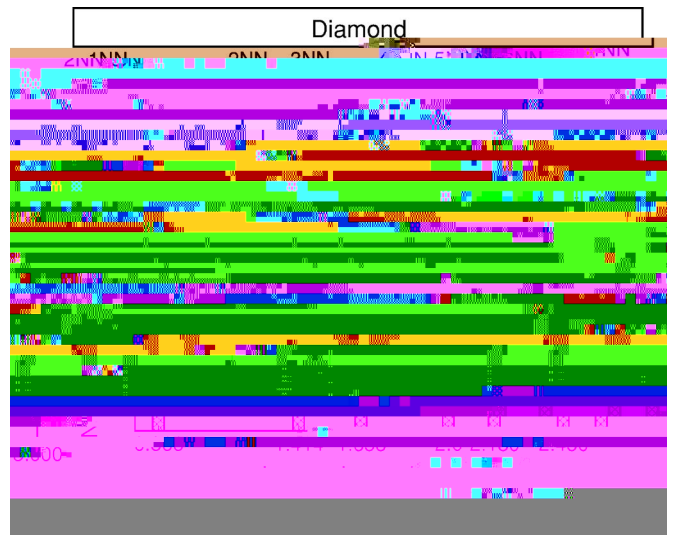
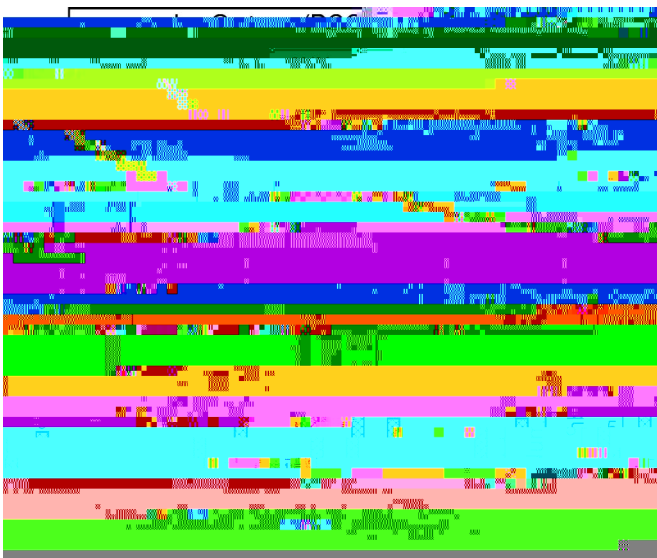
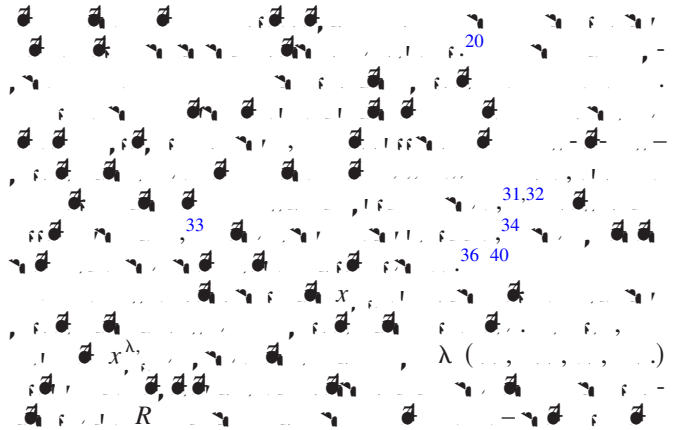
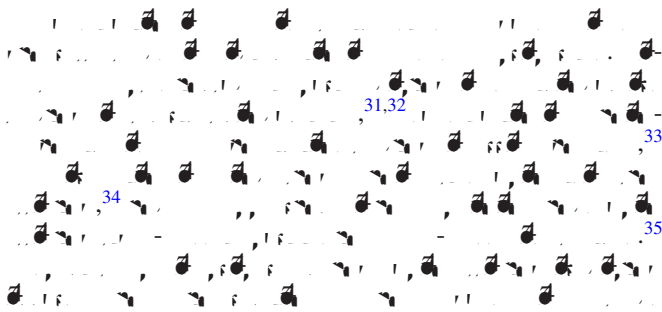


FIG. 7. (Color online) Percolation staircase on a lattice. The colors represent different clusters. The horizontal axis is the site index  $i$  and the vertical axis is the site index  $j$ .

FIG. 9. (Color online) Percolation staircase on a lattice. The colors represent different clusters. The horizontal axis is the site index  $i$  and the vertical axis is the site index  $j$ .

$R$  (34)  
 $H$  (5, 15) (6,41,42)  
 $x^\lambda$   
 $(\dots)$  (43,44)  
 $x$   
 $\in$   
 $M$   
 $M$   
 $(\dots)x^\lambda$  (45)  
 $R$  (20)  
 $R$  (33)  
 $R$  (6,41,42)  
 $x^\lambda$   
 $x^\lambda$   
 $M$   
 $R$   
 $R_1, R_2, R$



$\lambda = \lambda_1 \cup \dots \cup \lambda_k$  where  $\lambda_i \in \mathcal{P}(\{1, \dots, M\})$ .

...  $x_1, \dots, x_k$  ...  $\lambda$  ... [11](#).

1. ...  $k$ , ... **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. ...  $R$ , ...  $D$ , ...  $S$ , ... ( ) (1964).
15. ...  $T$ , ...  $y$ , ...  $D$ , ...  $S$ , ... ( ) (1975).
16. ... **16**, 1209 (1975).
17. ... H. ... **7**