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Defect dipoles and spontaneous polarization in acceptor doped ferroelectrics: Switching and interaction

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FG Mechanik funktionaler Materialien

FB Material- und Geowissenschaften

TU Darmstadt

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MECHANICS of FUNCTIONAL MATERIALS

Outline

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- Overview of Porject C6
- Recent results: influence of defect dipole
  - Phase field model
  - Simulation results
- Summary

Overview of the project C6

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In phase field modeling of ferroelectrics, we consider oxygen vacancies

- along with substitutions as static defect dipoles (ICCM 2012).
- or as switchable defect dipoles (current work).
- as stationary donors including other point defects (JAP, 115 (8); JAP, 116 (4))
- as diffsusing donors (current work).

Overview of the project C6

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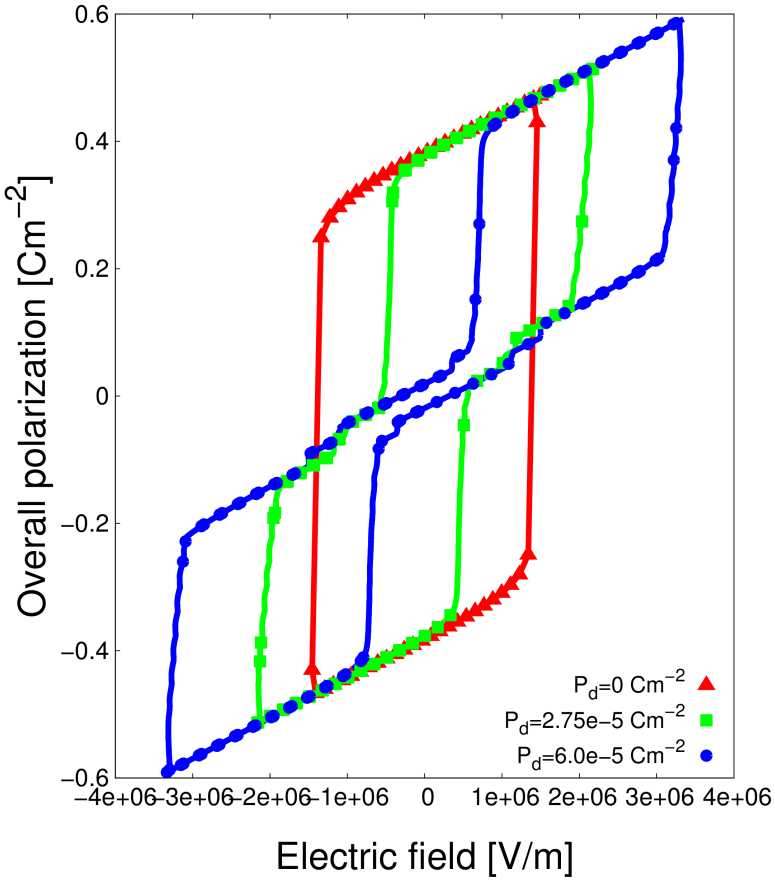

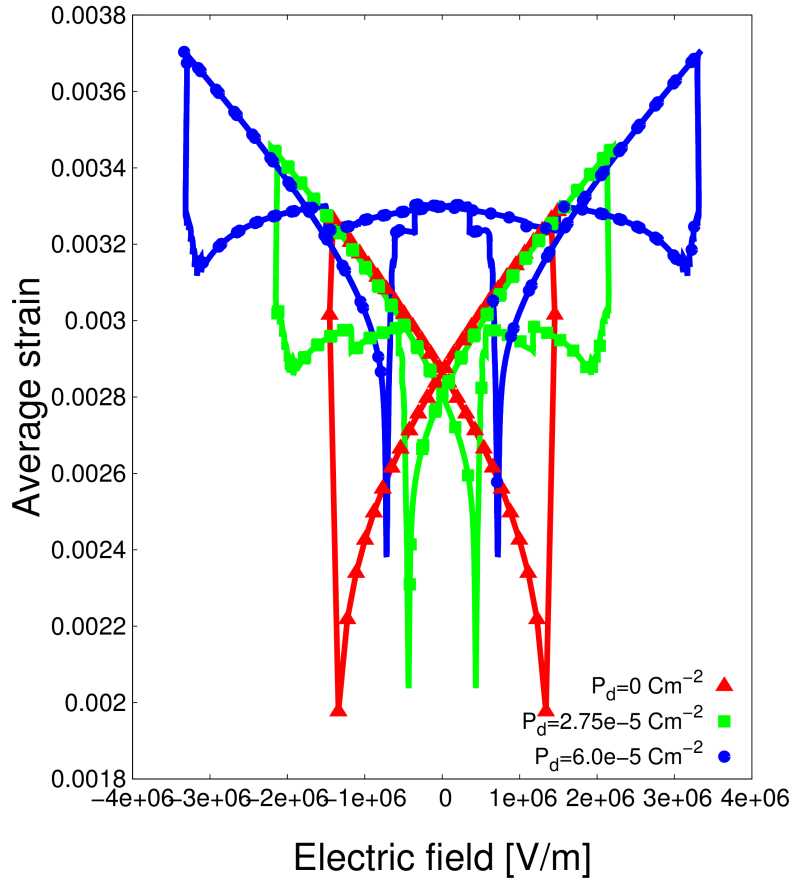

Zuo, Stein and Xu, ICCM Proceeding, 2012.

Overview of the project C6

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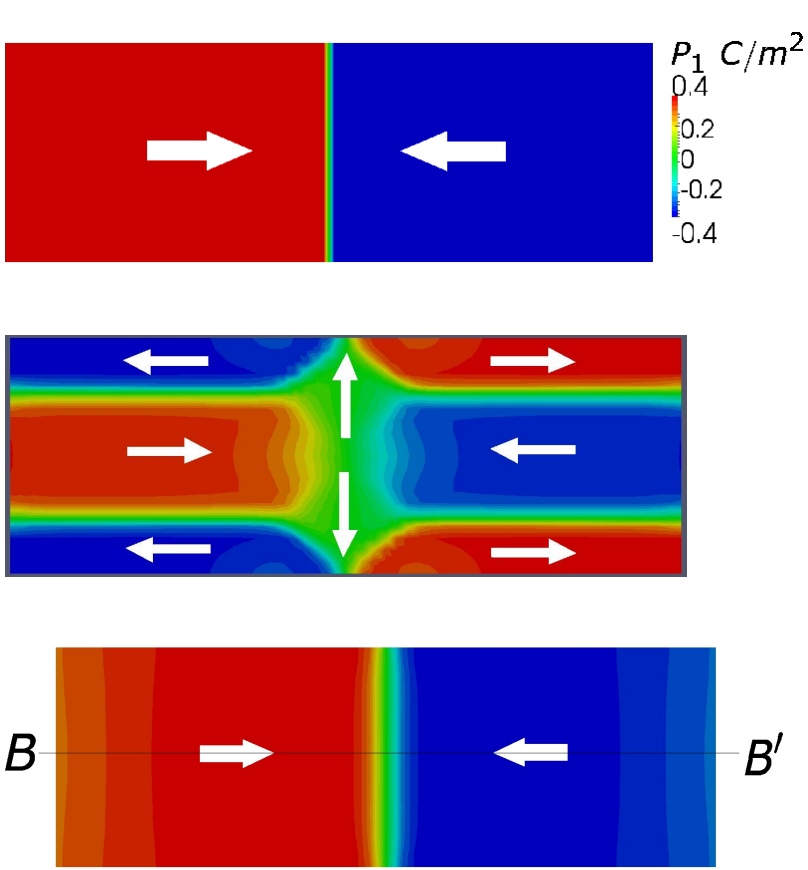

Zuo, Genenko, Klein, Stein and Xu, J. Appl. Phys., 2014.

Overview of the project C6

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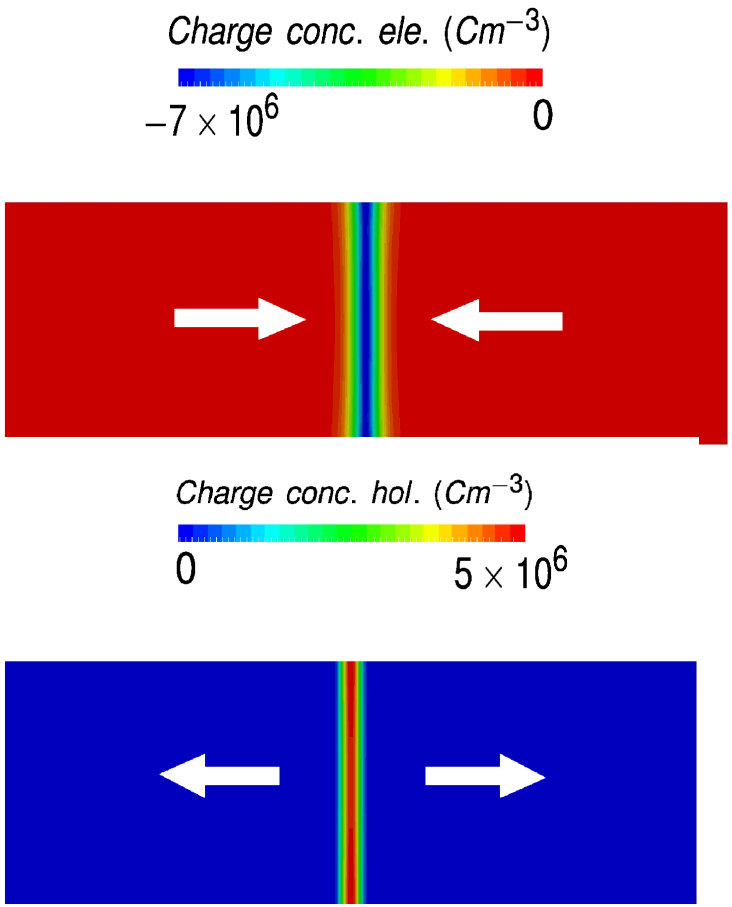

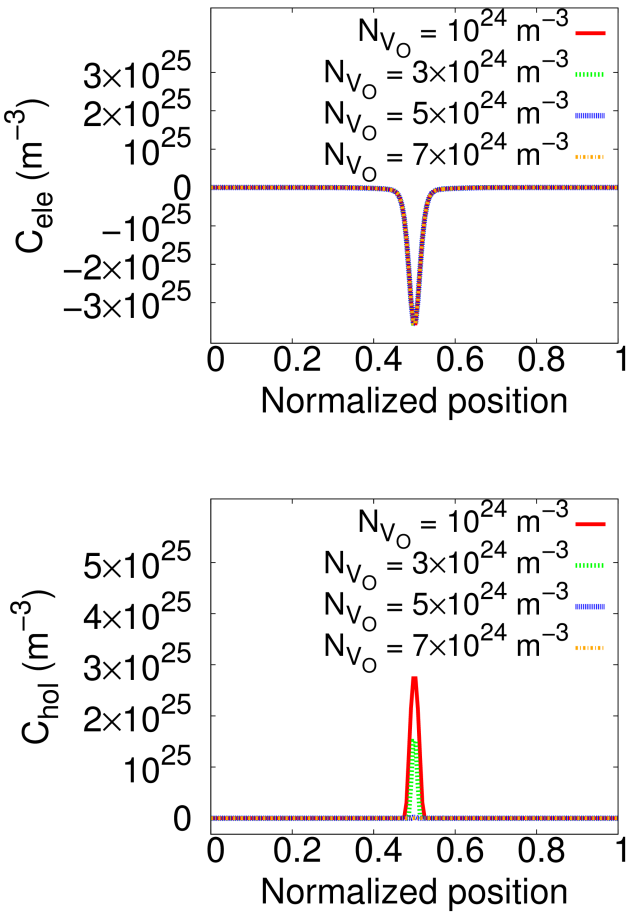

Zuo, Genenko and Xu, J. Appl. Phys., 2014.

Local defect polarization

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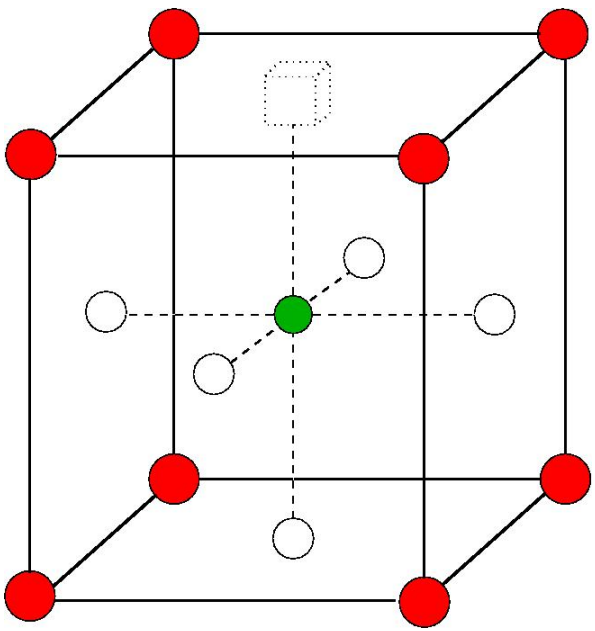

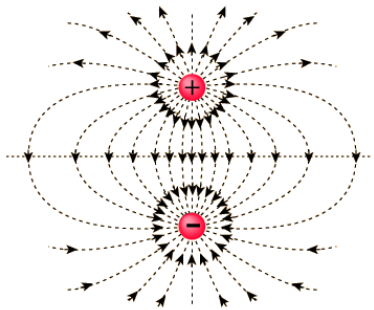

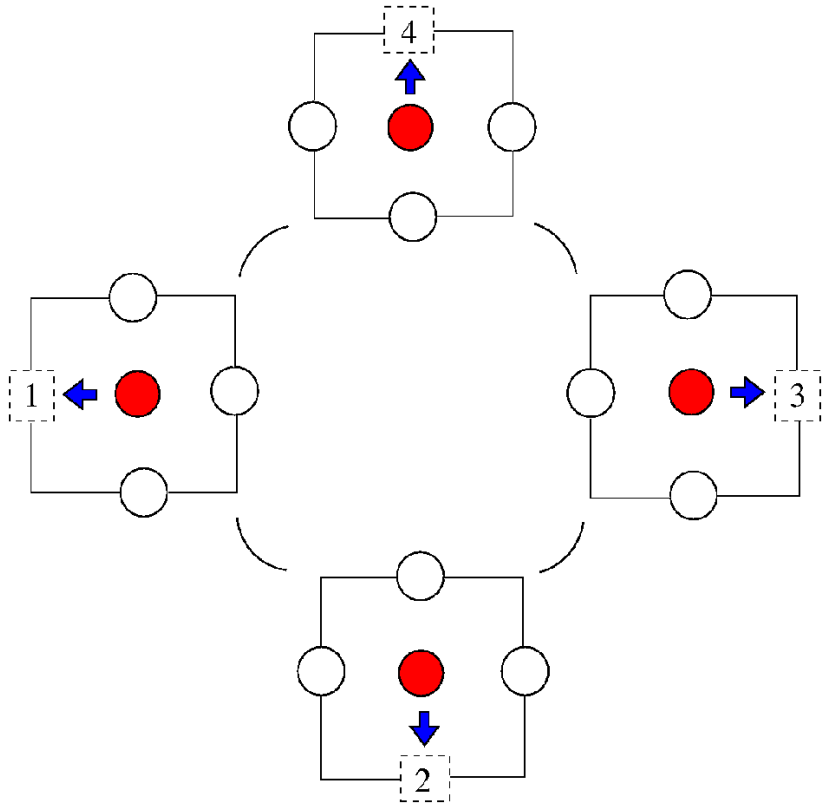

Concentration of each species $C_\alpha, \alpha = 1, 4$

Phase field model

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Total Gibbs energy

$$H = H^{ent}(S_{ij}, E_i^t, P_i^t) + H^{sep}(P_i^s) + H^{grad}(P_{i,j}^s).$$

$$H^{ent} = \frac{1}{2}(S_{ij} - S_{ij}^0)C_{ijkl}(S_{kl} - S_{kl}^0) - (S_{ij} - S_{ij}^0)b_{kij}E_k^t - \frac{1}{2}E_i^t\varepsilon_{ij}E_j^t - P_i^tE_i^t$$

$$H^{sep} = \frac{\kappa_s G}{\epsilon}[a_1 + a_2(P_1^{s2} + P_2^{s2}) + a_3(P_1^{s4} + P_2^{s4}) + a_4P_1^{s2}P_2^{s2} + a_5(P_1^{s6} + P_2^{s6})]$$

$$H^{grad} = \kappa_i\frac{G\epsilon}{P_0^2}(P_{1,1}^{s2} + P_{1,2}^{s2} + P_{2,1}^{s2} + P_{2,2}^{s2})$$

Phase field model

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Constitutive laws

$$D_i = -\frac{\partial H}{\partial E_i} = b_{ijk}(S_{jk} - S^0_{jk}) + A_{ij}E^t_j + P^s_i + P^d_i$$

$$\sigma_{ij} = \frac{\partial H}{\partial S_{ij}} = C_{ijkl}(S_{kl} - S^0_{kl}) - b_{kij}E^t_k$$

$$E^t_i = E^e_i + E^d_i, E^d_i = \frac{C_0 P^d_i}{\pi \kappa_0}$$

(Eichel et al., Phys. Rev. Lett., 2008)
Evolution of spontaneous polarization

$$\frac{\partial P^s_i}{\partial t} = -M\frac{\delta H}{\delta P^s_i}$$

Local defect polarization

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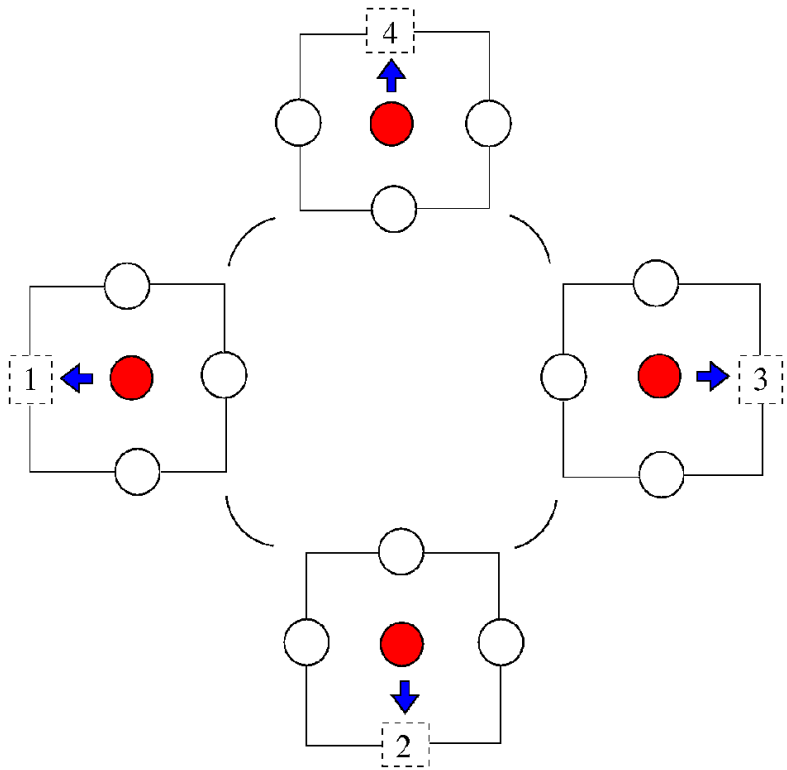

$$P_i^d = (c_{i+2} - c_i)\, V_0 P_0^d$$

Temporal evolution of concentration of oxygen vacancies

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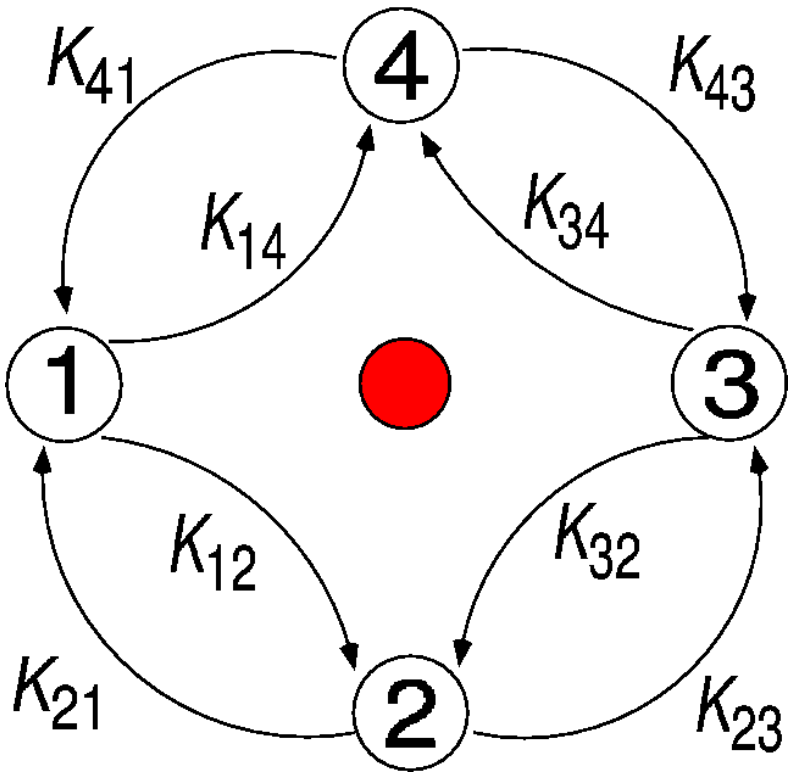


$$\dot{c}_1 = -\frac{1}{2}K_{12}c_1 - \frac{1}{2}K_{14}c_1 + \frac{1}{2}K_{21}c_2 + \frac{1}{2}K_{41}c_4$$

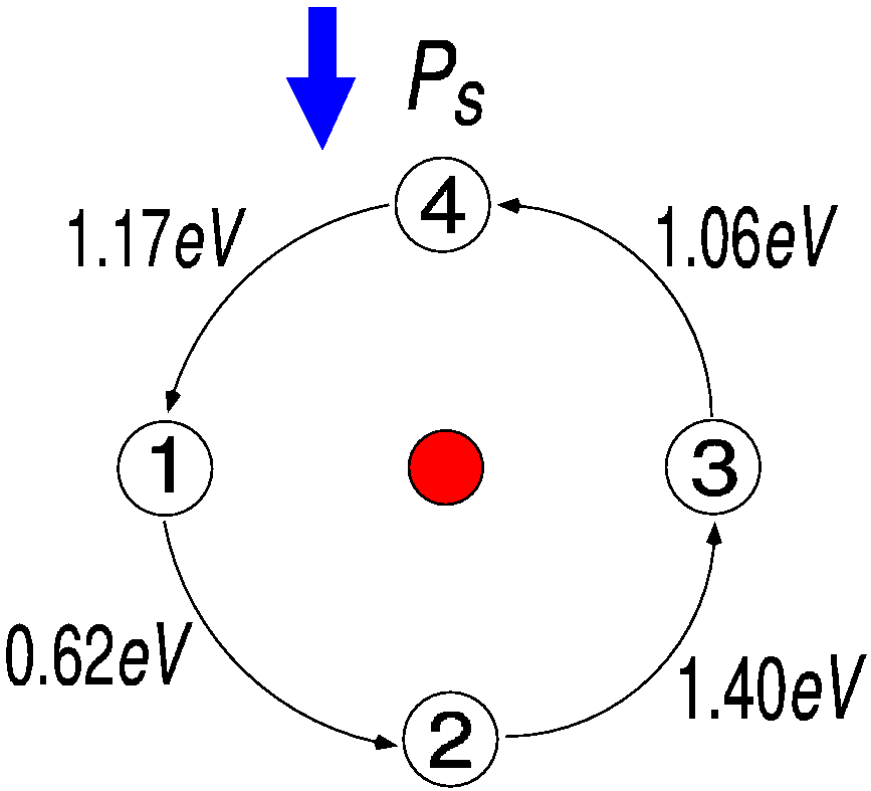
$$\dot{c}_2 = -\frac{1}{2}K_{23}c_2 - \frac{1}{2}K_{21}c_2 + \frac{1}{2}K_{32}c_3 + \frac{1}{2}K_{12}c_1$$

$$\dot{c}_3 = -\frac{1}{2}K_{34}c_3 - \frac{1}{2}K_{32}c_3 + \frac{1}{2}K_{43}c_4 + \frac{1}{2}K_{23}c_2$$

$$\dot{c}_4 = -\frac{1}{2}K_{41}c_4 - \frac{1}{2}K_{43}c_4 + \frac{1}{2}K_{14}c_1 + \frac{1}{2}K_{34}c_3$$

(Erhart, Träskelin and Albe, Phys. Rev. B. 2013)

Temporal evolution of concentration of oxygen vacancies



$$K_{ij} = \nu exp(-\frac{\Delta E_{i-j}}{k_B T})$$

At room temperature, the switching takes several days

At 450K the switching completes within minutes

Evolution of oxygen vacancies and spontaneous polarization

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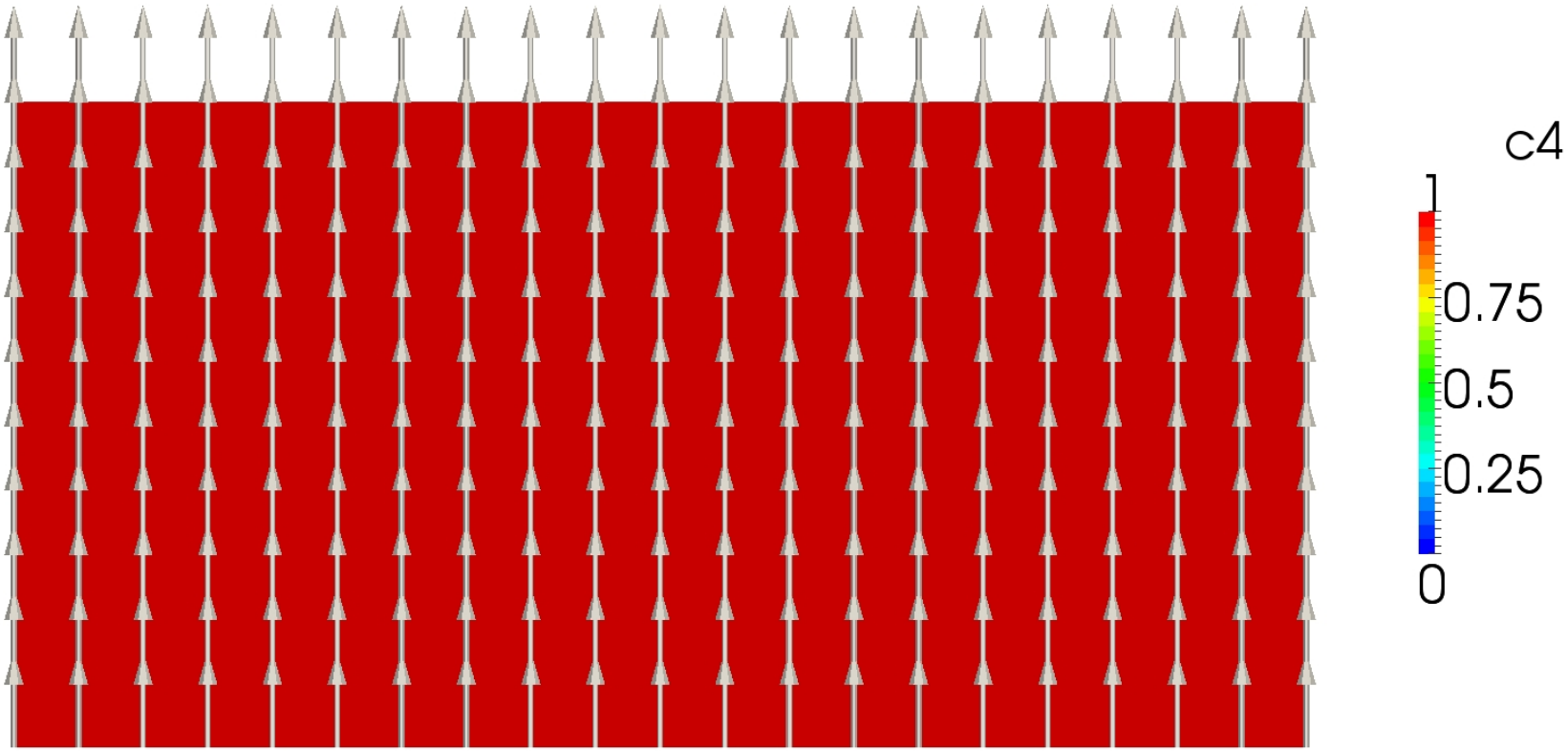

Evolution of oxygen vacancies and spontaneous polarization

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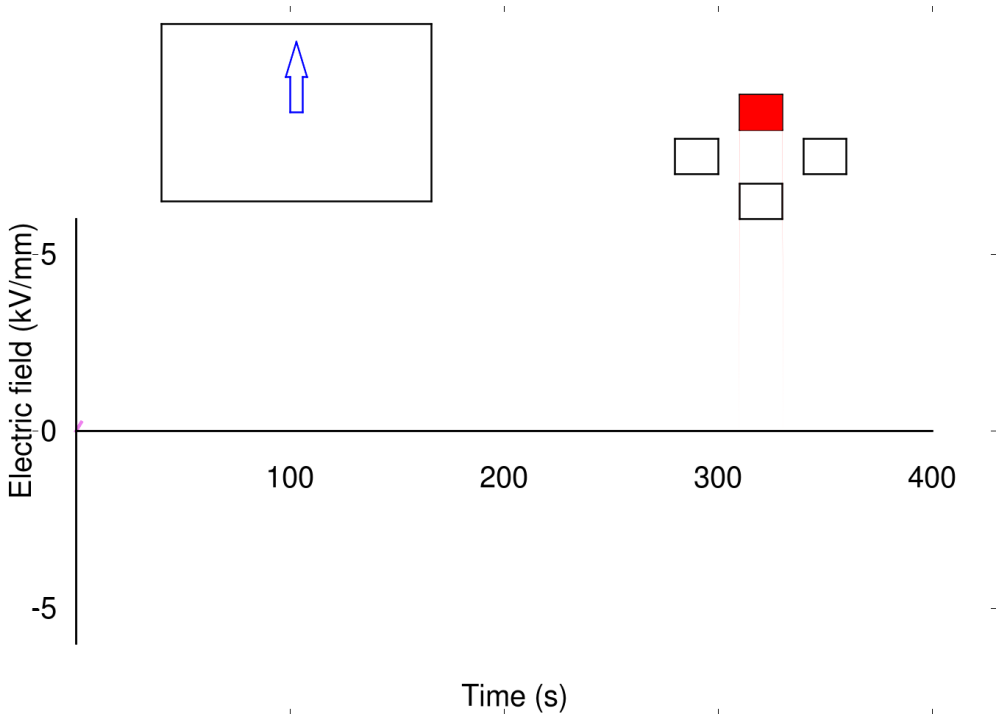

Summary

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- **Implementation of the switching of defect dipoles**
  - Defect dipole can be switched in minutes at high temperature
  - Larger electric field necessary for switching
- **To be considered**
  - Mechanism of aging due to defect dipoles

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Thank you!