

Enhanced Piezoelectricity in Relaxor Ferroelectrics: A Phenomenological Approach

J. –M. Liu (刘俊明), L. F. Wang

Email: liujm@nju.edu.cn

<http://pld.nju.edu.cn>

**Department of Physics, Nanjing University
Nanjing National Laboratory of Microstructures**



OUTLINES

Introduction & Motivation

Model & Simulation

Results

- Domain Patterns
- Energy Terms
- Field Enhanced Piezoelectricity
- Enhanced Piezoelectricity at Zero Field
- Enhanced Piezoelectricity: Critical Phenomena

Summary

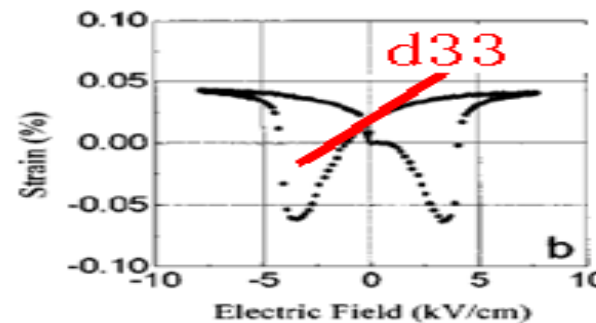
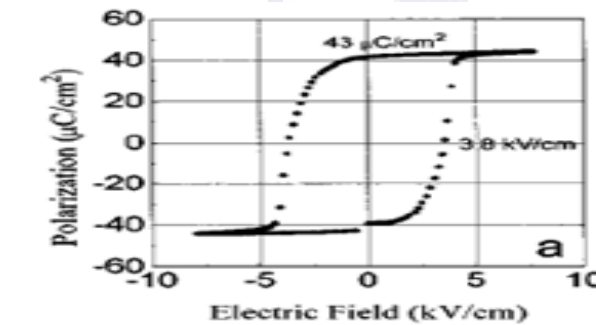


Introduction & Motivation:

Principle

Polarization

Strain



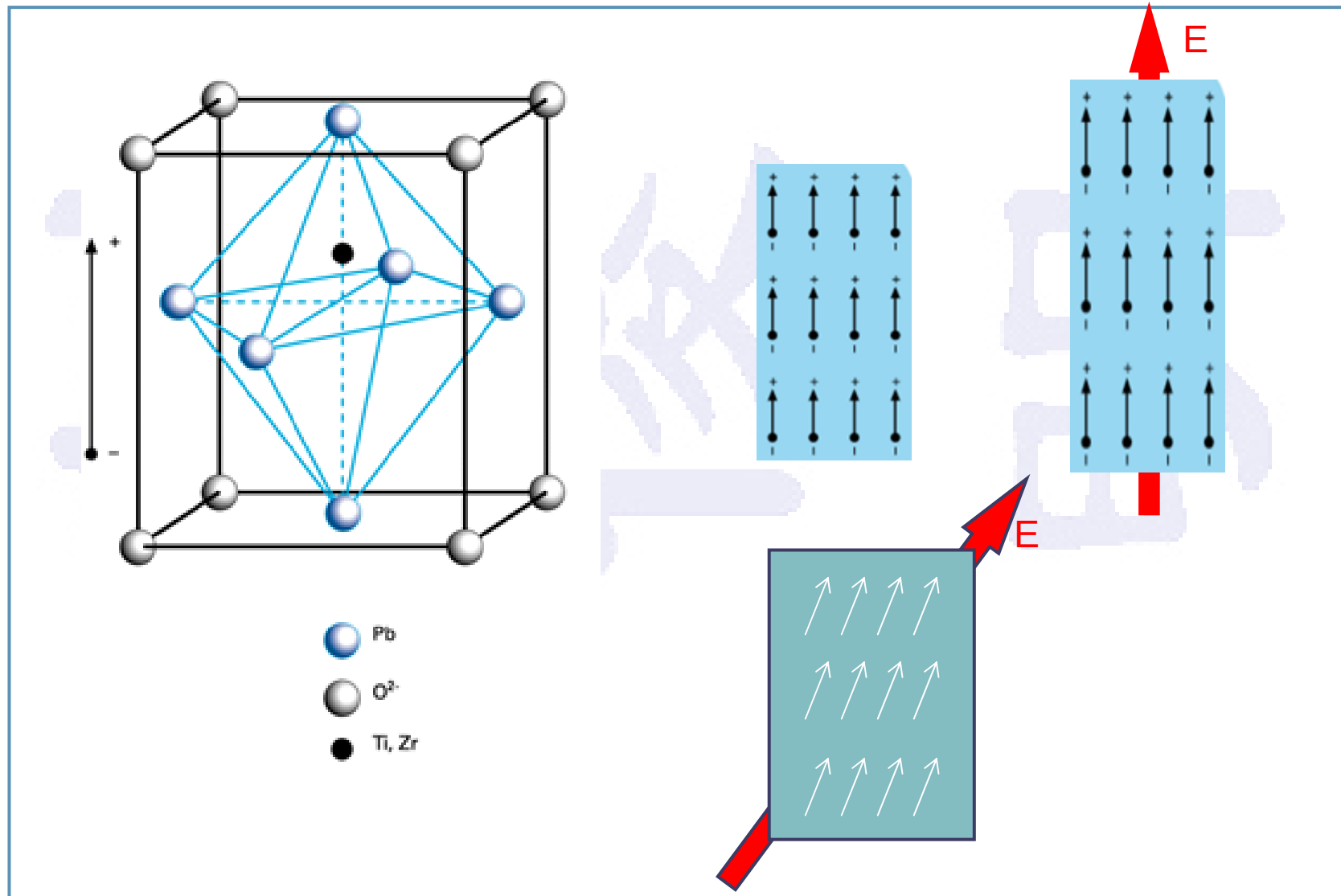
Electrical
energy

Mechanical
energy



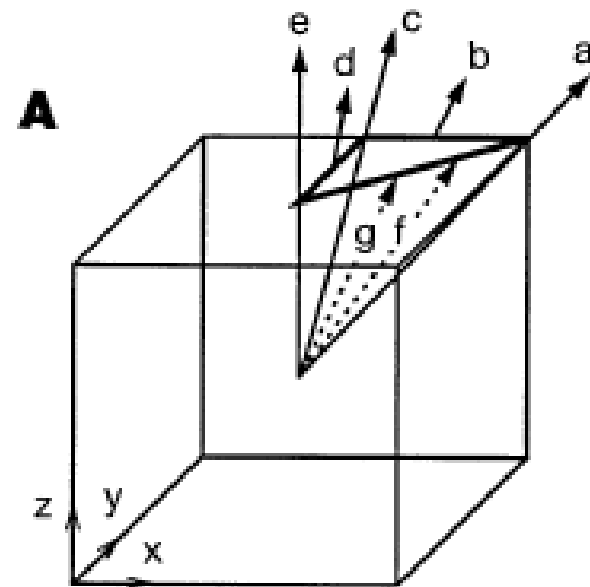
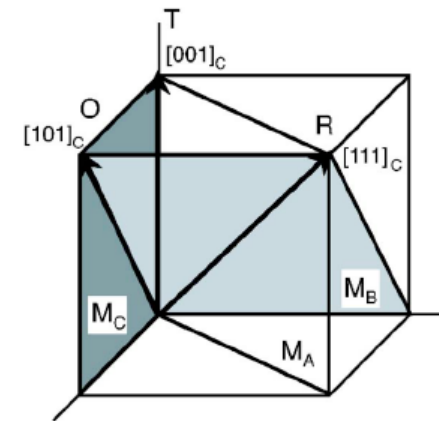
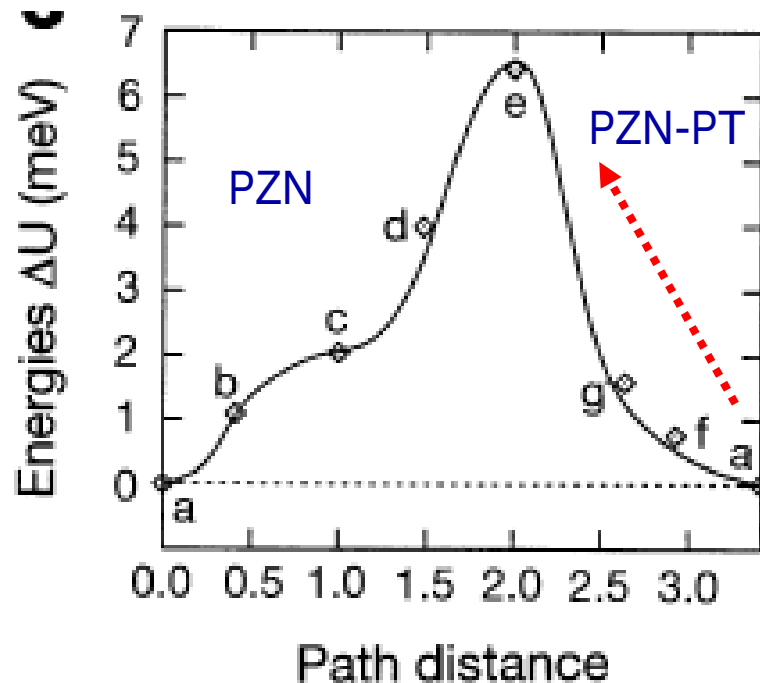
Introduction & Motivation

Polarization rotation $\Rightarrow$ piezoelectricity



Introduction & Motivation

Polarization rotation $\Rightarrow$ first-principle calculation

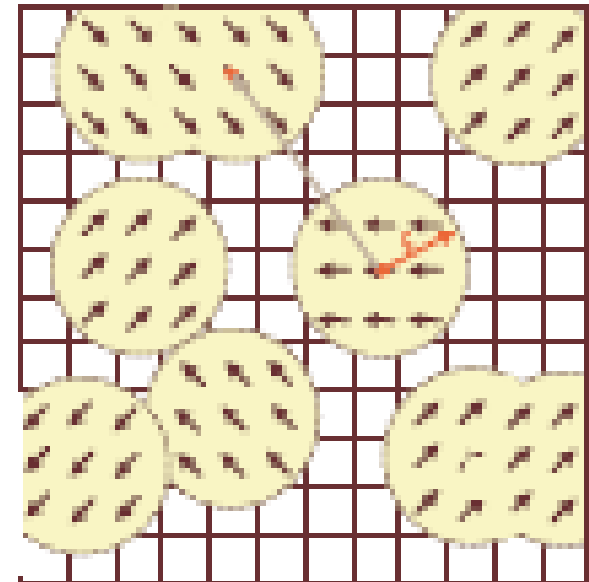
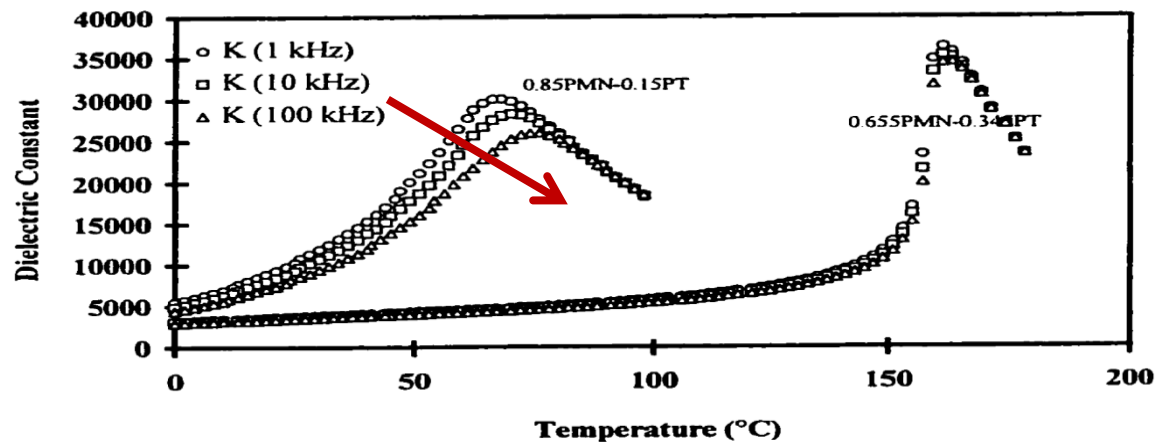
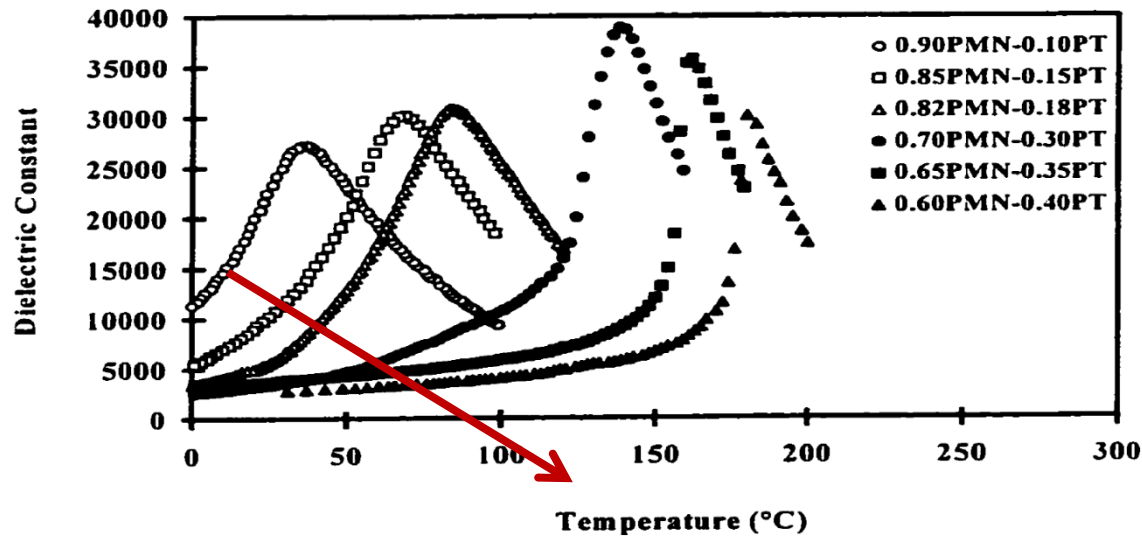


H.Fu, R.E.Cohen, Nature 403, 281 (2000)



Introduction & Motivation

Relaxors $\Rightarrow$ dielectric response & enhanced ferroelectricity



J. M. Kelly, PhD dissertation (1998). {A. Safari, Rutgers}

Introduction & Motivation

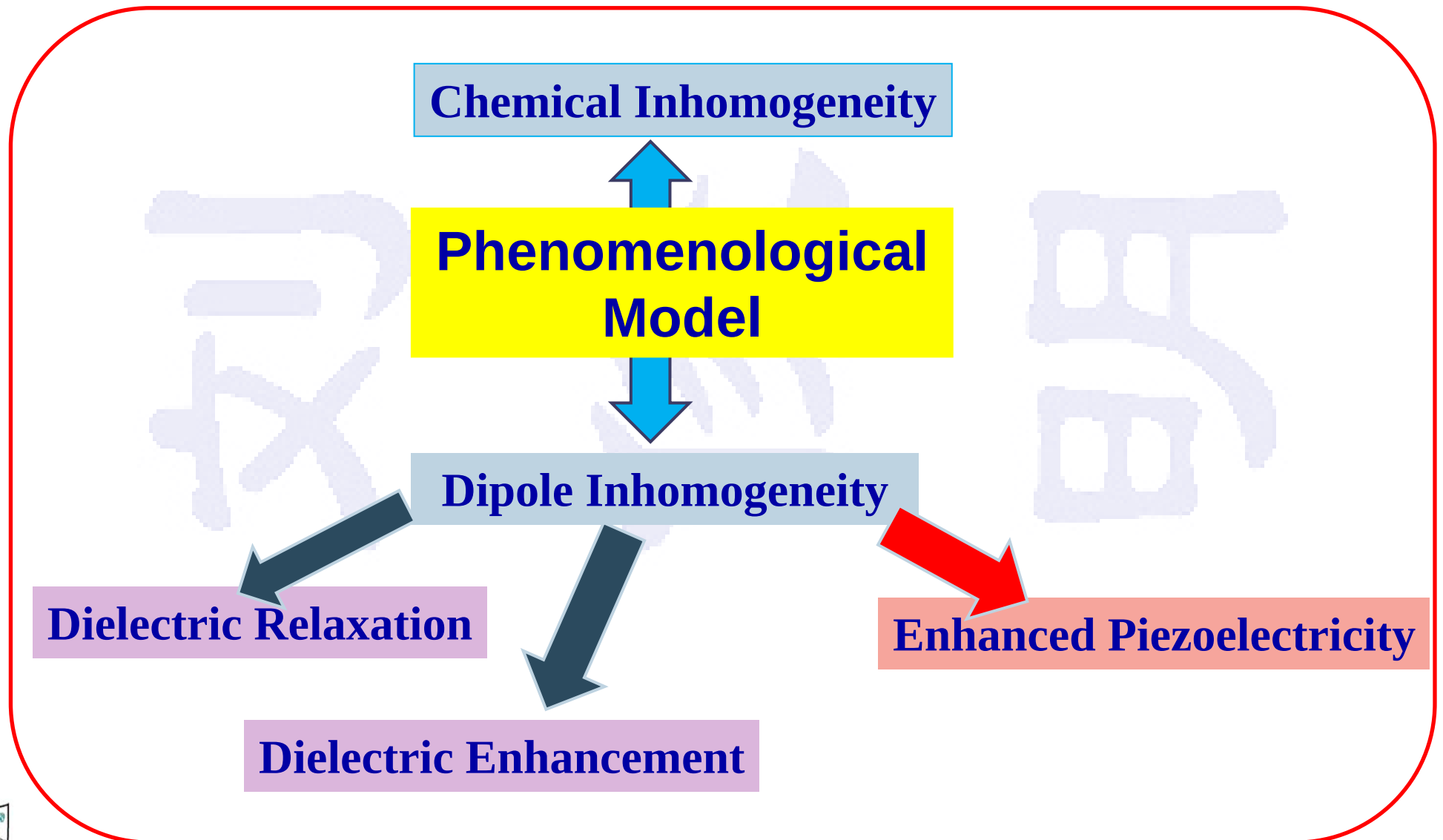
Problems in relaxors:

- 1. Polarization rotation induced piezoelectricity enhancement?**
- 2. Ferroelectric nanoclusters induced piezoelectricity enhancement?**



Model and simulation

Strategy:



Model and simulation: two-dimensional model

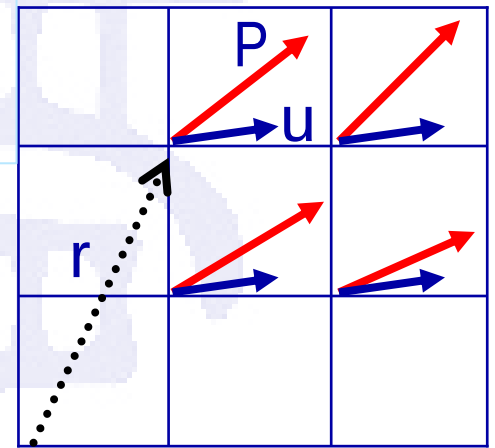
$$F[\vec{P}(\vec{r}), \vec{u}(\vec{r})] = \int_{\Omega} \{f_p + f_g + f_u + f_c + f_E\} \cdot d\vec{r}$$

$$f_p(\vec{P}(\vec{r})) = A_I(P_x^2 + P_y^2) + A_{II}(P_x^4 + P_y^4) + A_{I2}P_x^2P_y^2 \\ + A_{III}(P_x^6 + P_y^6) + A_{II2}(P_x^4P_y^2 + P_y^4P_x^2),$$

$$A_I(\mathbf{r}) = A_0(T - T_0) + b_m(\mathbf{r}) \cdot C(\mathbf{r}) + \sum_R \{s(\mathbf{r} + \mathbf{R})\}$$

$$s(\mathbf{r} + \mathbf{R}) = b_m(\mathbf{r} + \mathbf{R}) \cdot C(\mathbf{r} + \mathbf{R}) \cdot R^{-a}$$

$$C_0, C_p, b_M, T, T_0, a$$



Model and simulation: two-dimensional model

$$f_g(P_{i,j}) = \frac{1}{2} [G_{11}(P_{x,x}^2 + P_{y,y}^2) + G_{12}P_{x,x}P_{y,y} + G_{44}(P_{x,y} + P_{y,x})^2 + G_{44}(P_{x,y} - P_{y,x})^2]$$

$$P_{i,j} = \partial P_i / \partial r_j$$

$$f_u(u_{i,j}) = \frac{1}{2} C_{11}(u_{x,x}^2 + u_{y,y}^2) + C_{12}u_{x,x}u_{y,y} + \frac{1}{2} C_{44}u_{x,y}^2,$$

$$u_{ii} = \partial u_i / \partial r_i, \quad u_{i,j} = \partial u_j / \partial r_i + \partial u_i / \partial r_j$$

$$f_c(u_{i,j}, \vec{P}(\vec{r})) = -u_{x,x}\eta_{xx} - u_{y,y}\eta_{yy} - u_{x,y}\eta_{xy}$$

$$\eta_{xx} = Q_{11}P_x^2 + Q_{12}P_y^2;$$

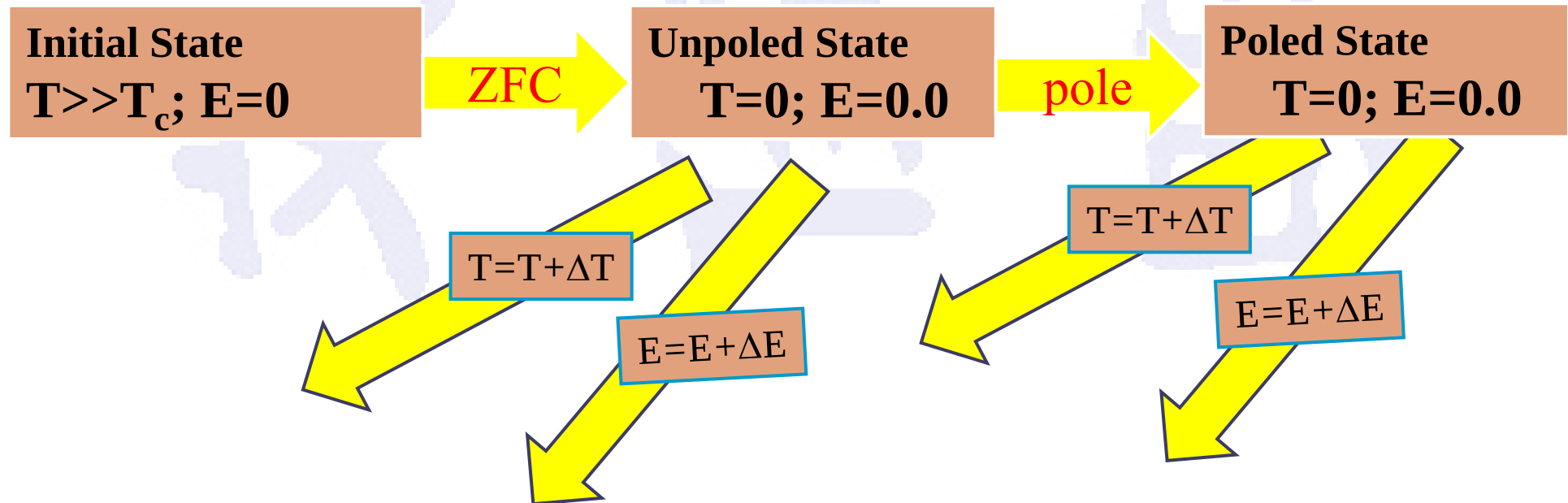
$$\eta_{yy} = Q_{11}P_y^2 + Q_{12}P_x^2; \quad \eta_{xy} = Q_{44}P_xP_y$$

$$f_E = -\vec{E} \cdot \vec{P}$$



Model and simulation: procedure

$$\begin{cases} \partial P_i(\mathbf{r}, t) / \partial t = -L_P \cdot \delta F / \delta P_i(\mathbf{r}, t), \\ \partial u_i(\mathbf{r}, t) / \partial t = -L_u \cdot \delta F / \delta u_i(\mathbf{r}, t), \end{cases} \quad (i=x, y)$$



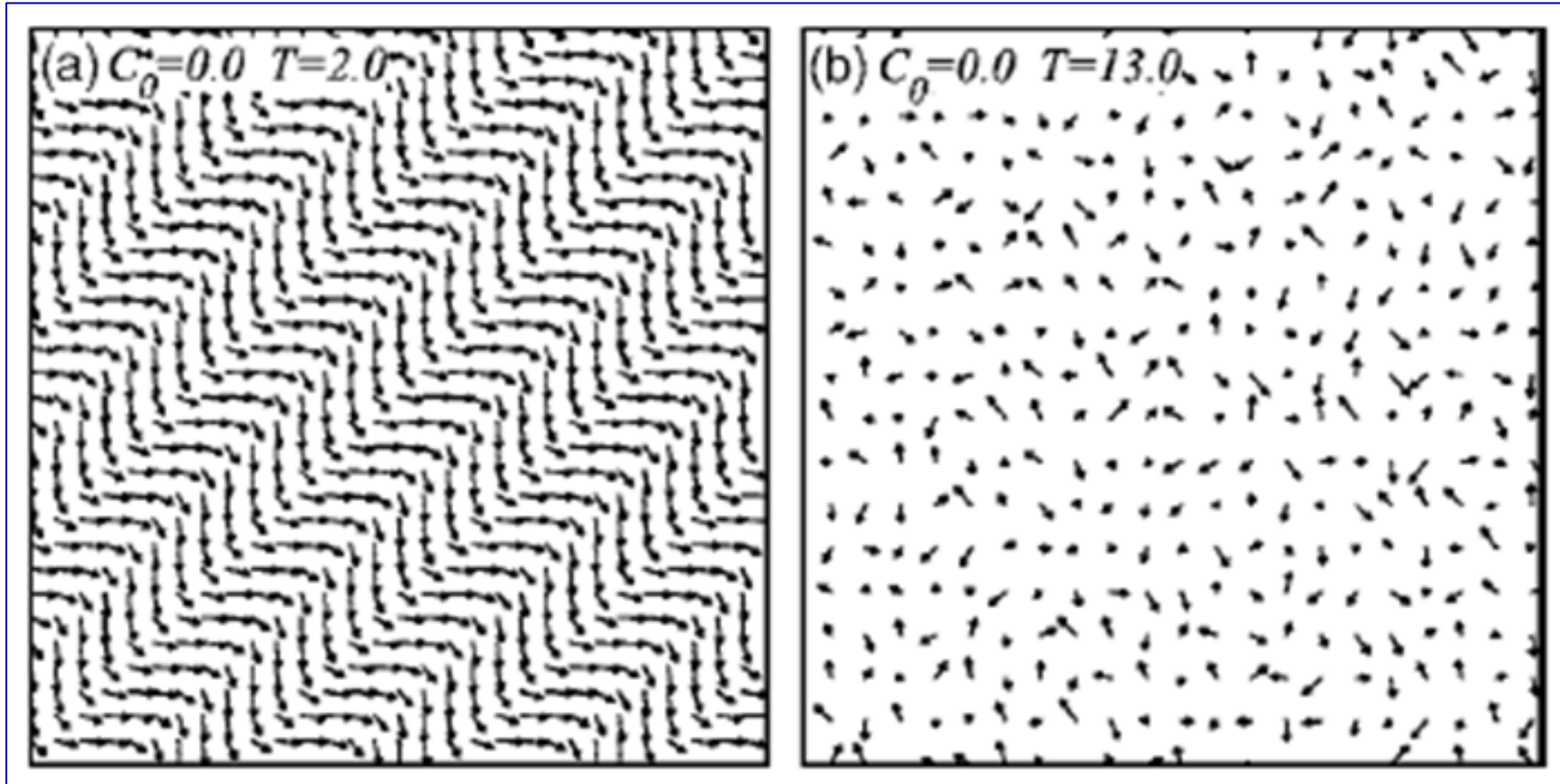
Results & discussion:

Normal ferroelectrics
or
Relaxor ferroelectrics



Results & discussion: domain patterns

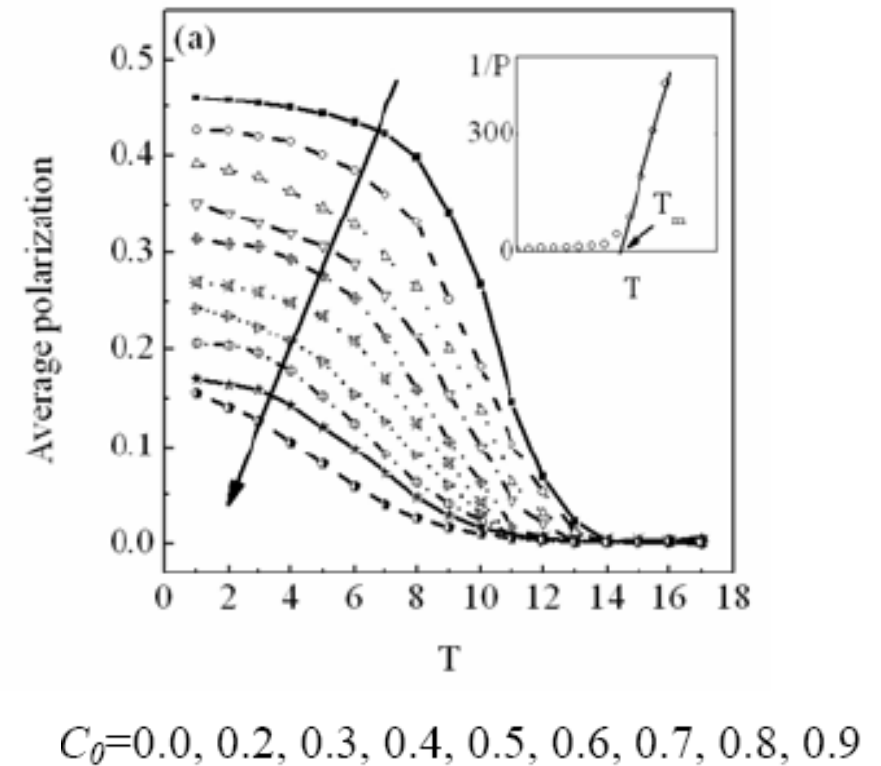
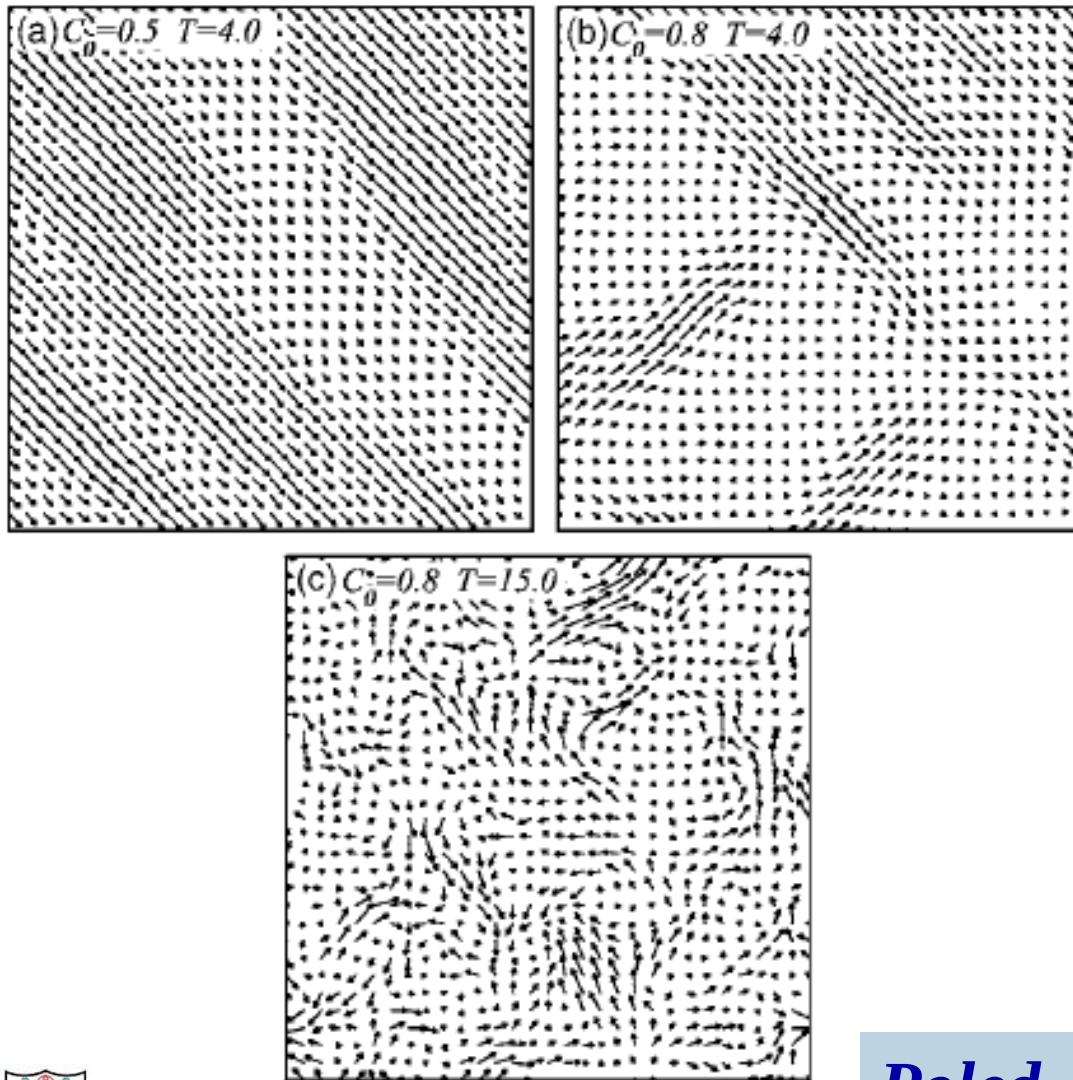
Normal ferroelectrics



$$T_0=10.0$$

Results & discussion: domain patterns

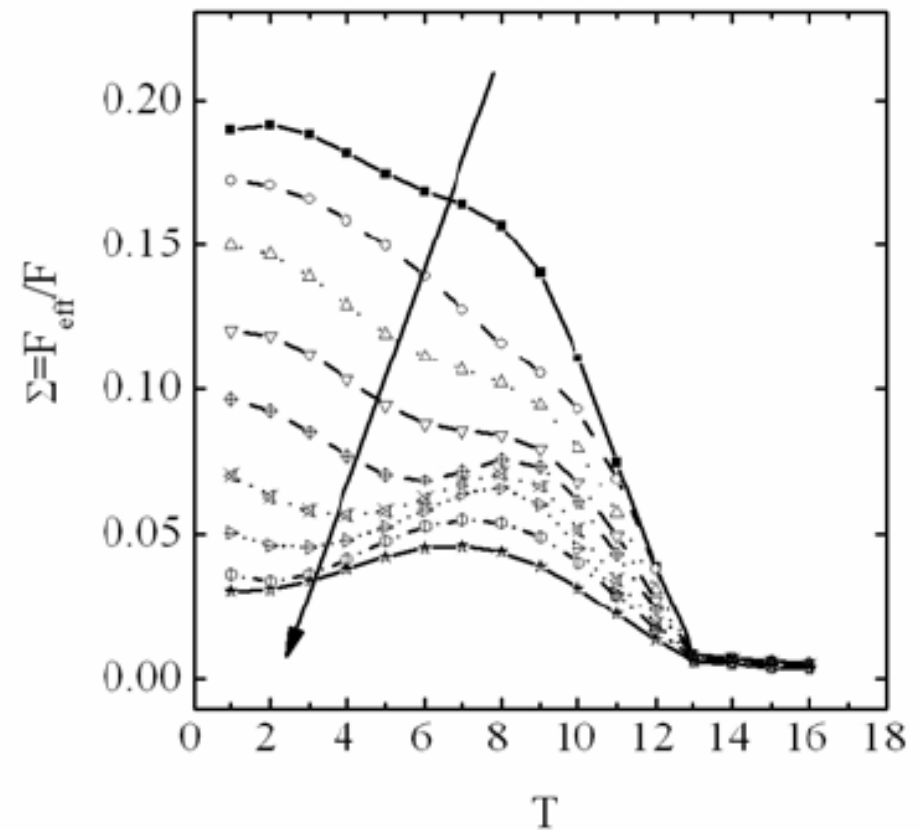
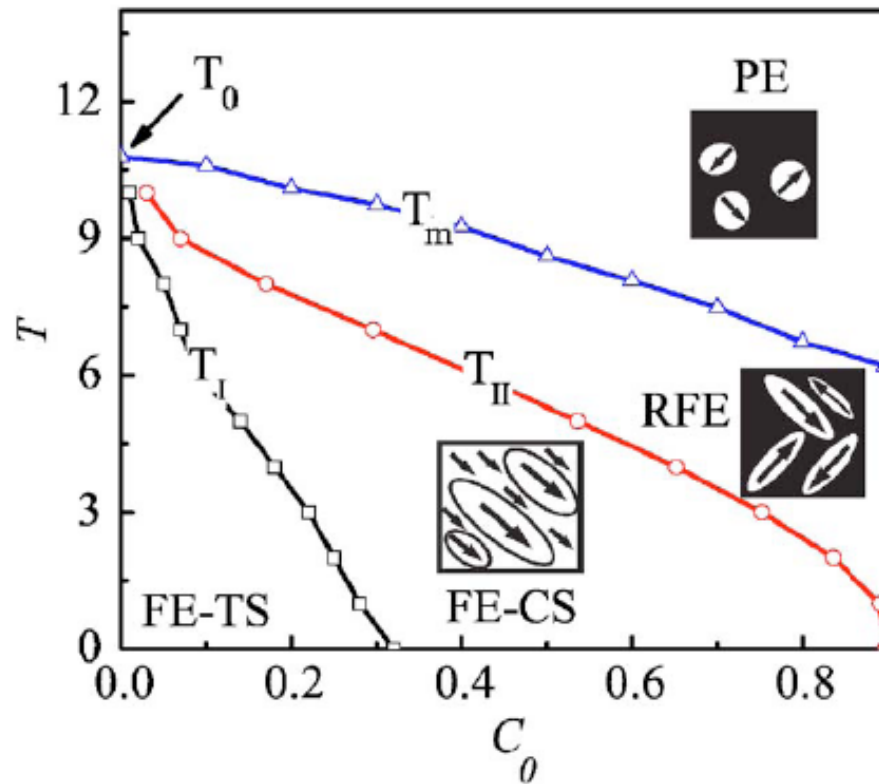
Relaxors



Poled, $C_p=0.5$, $b_M=6$, $T_c=10.0$, $a=1.5$

Results & discussion: energy terms

Phase diagram & elastic energy



$C_0=0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9$

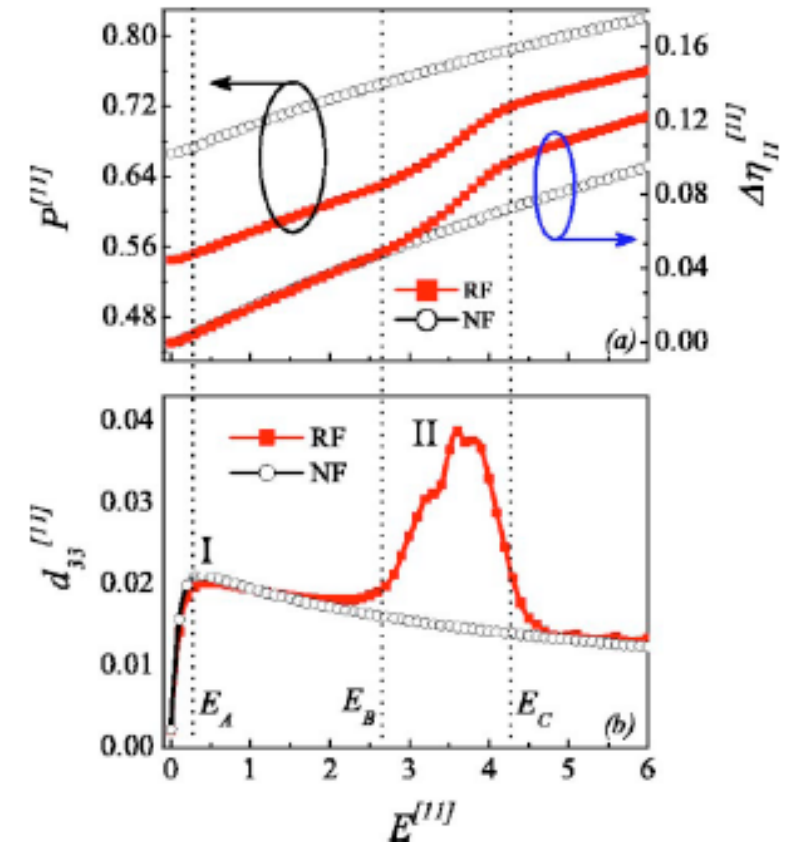
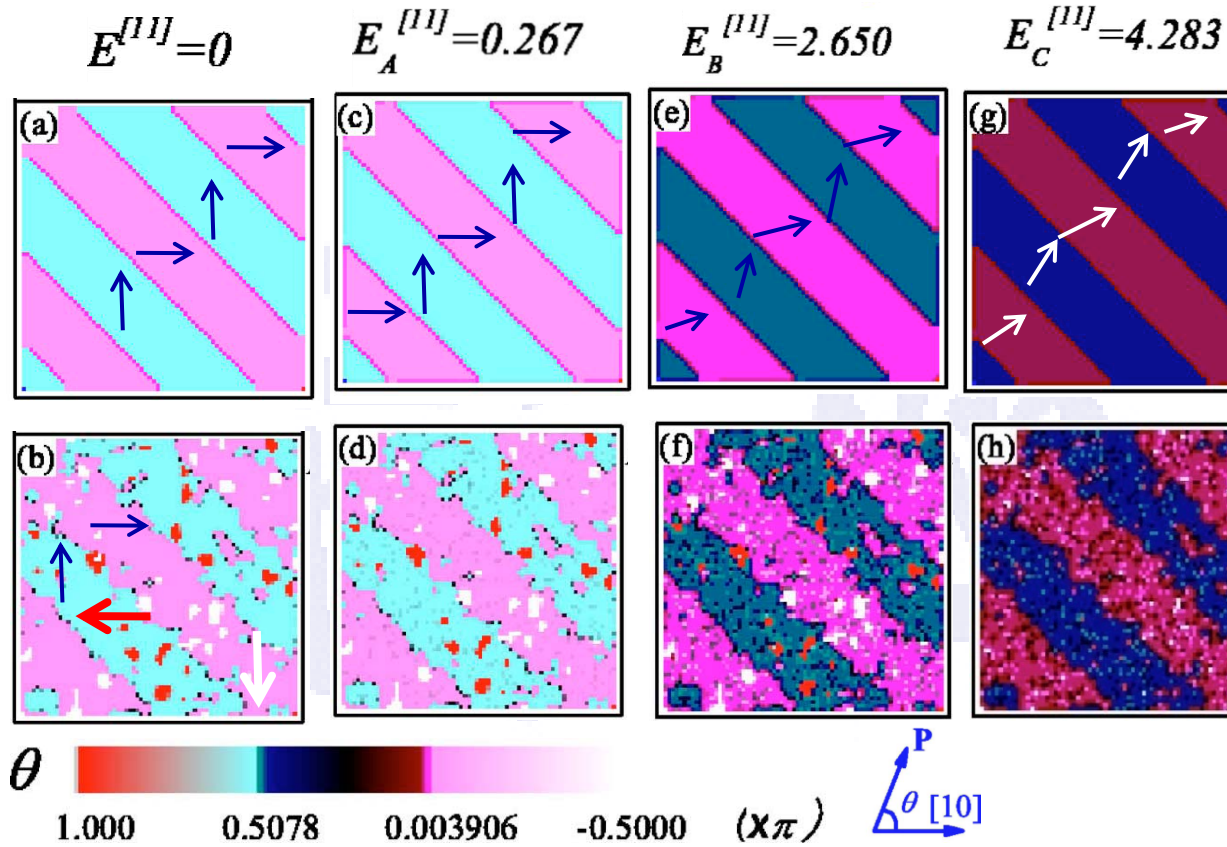
Results & discussion:

Field enhanced piezoelectricity in relaxors



Results & discussion: enhanced piezoelectricity

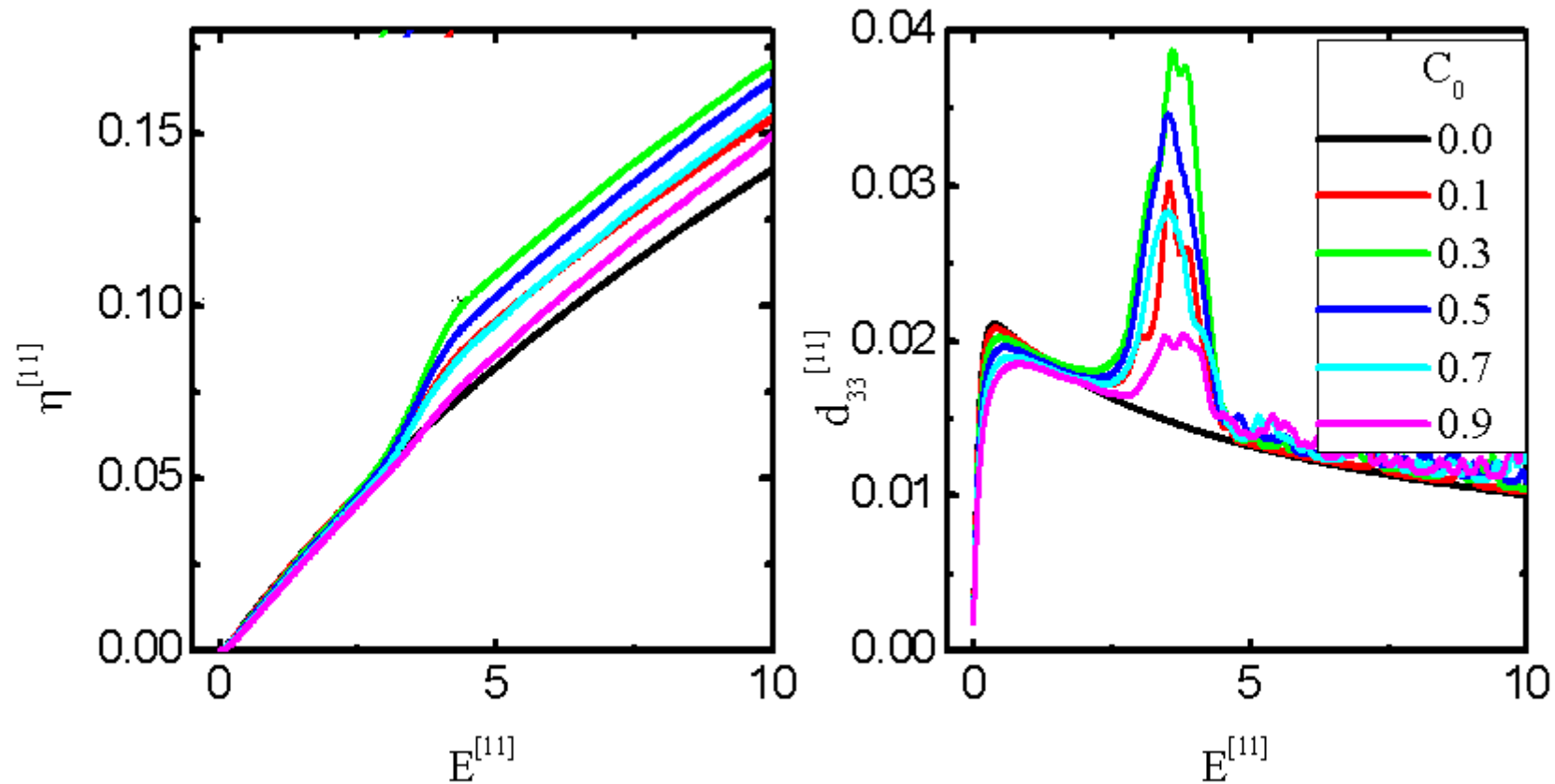
90°-domain flip



Unpoled, $C=0.3$, $C_p=0.5$, $b_M=25$, $T=1.0$, $T_c=10.0$, $a=\infty$

Results & discussion: enhanced piezoelectricity

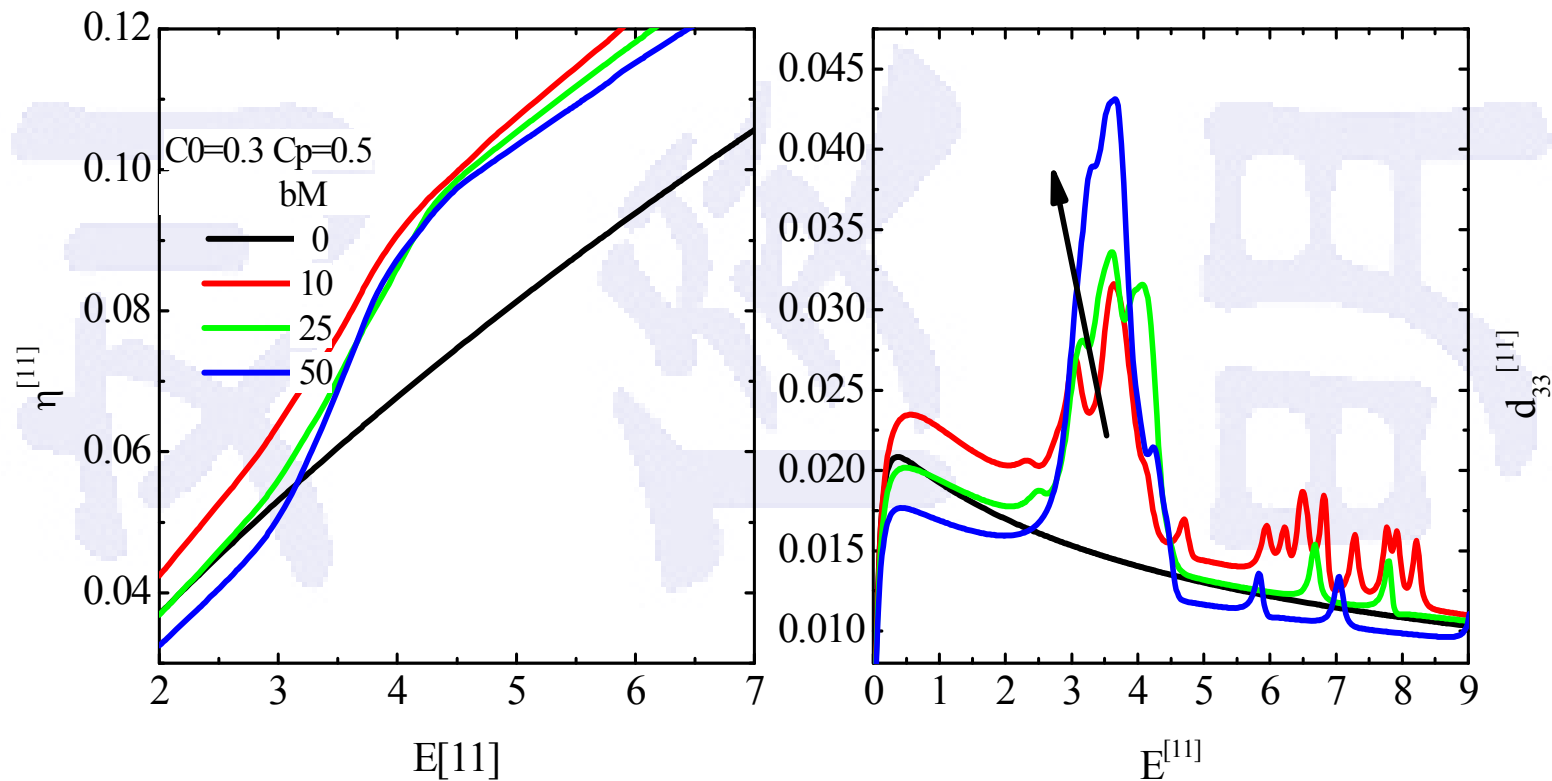
90°-domain flip



Unpoled, $C=0.3$, $C_p=0.5$, $b_M=25$, $T=1.0$, $T_c=10.0$, $a=\infty$

Results & discussion: enhanced piezoelectricity

90°-domain flip



Unpoled, $C=0.3$, $C_p=0.5$, $b_M=25$, $T=1.0$, $T_c=10.0$, $a=\infty$

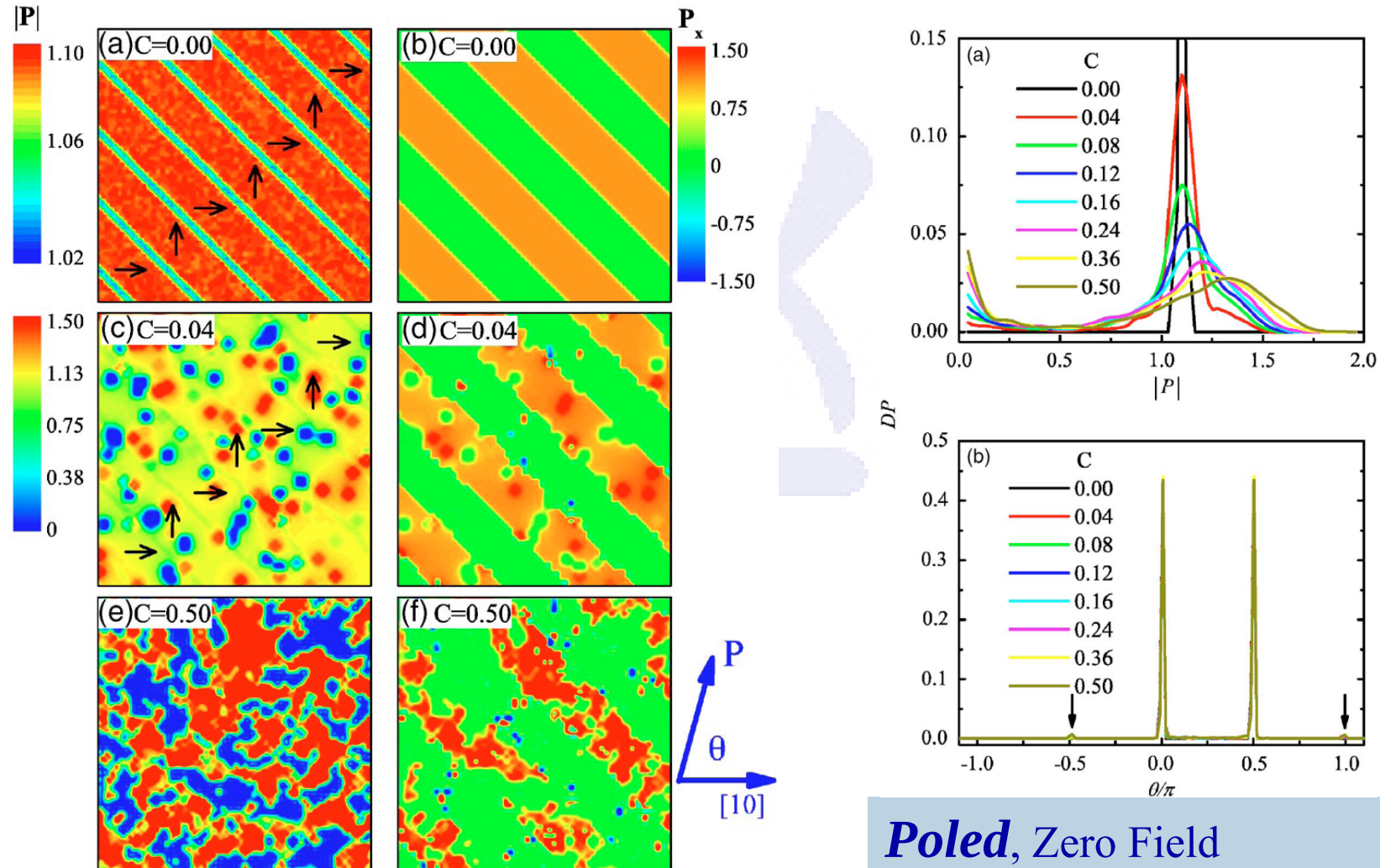
Results & discussion:

**Nanocluster enhanced
piezoelectricity in relaxors**



Results & discussion: enhanced piezoelectricity

Cluster size effect



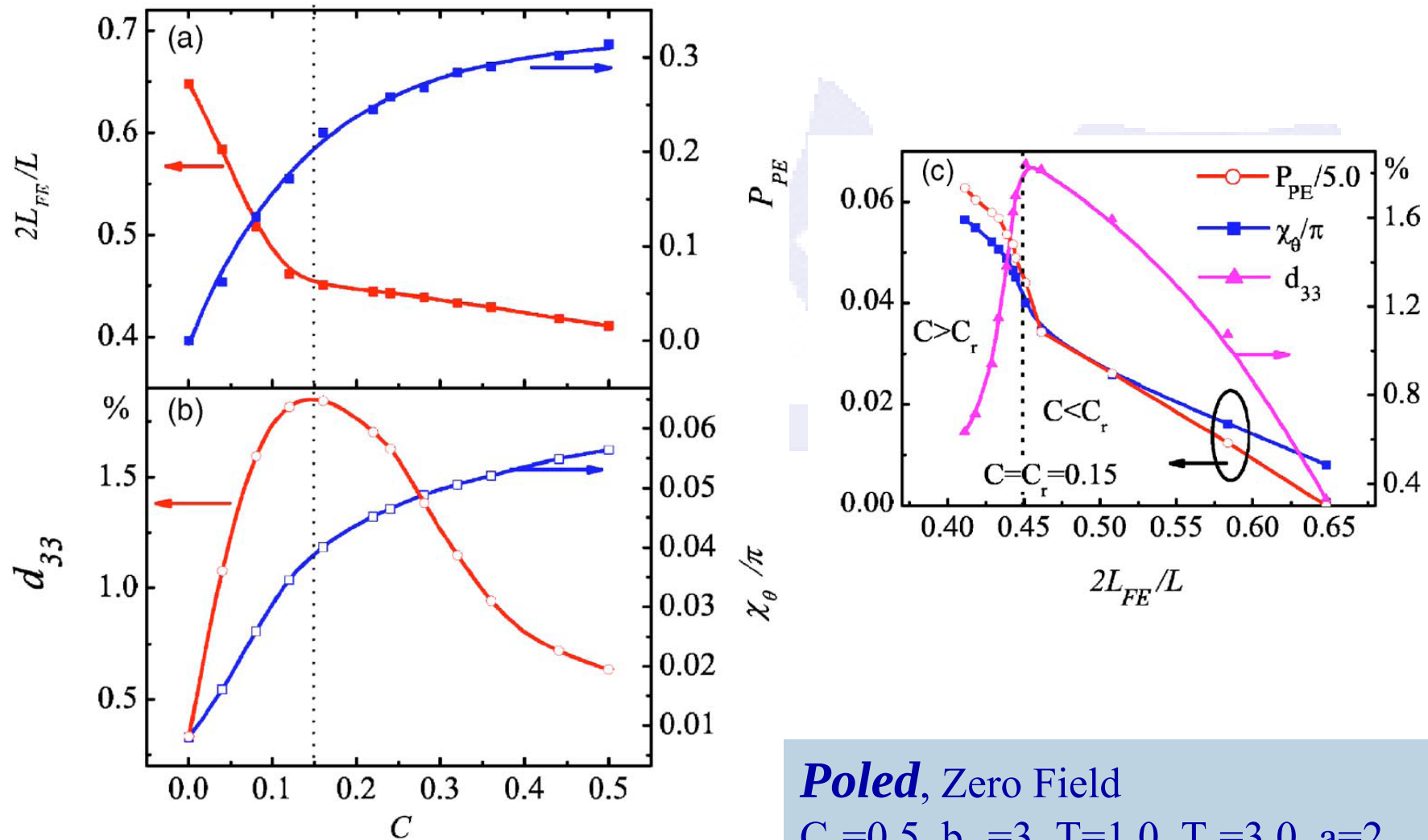
Poled, Zero Field

$C_p=0.5, b_M=3, T=1.0, T_c=3.0, a=2$



Results & discussion: enhanced piezoelectricity

Cluster size effect



Poled, Zero Field

$C_p=0.5, b_M=3, T=1.0, T_c=3.0, a=2$



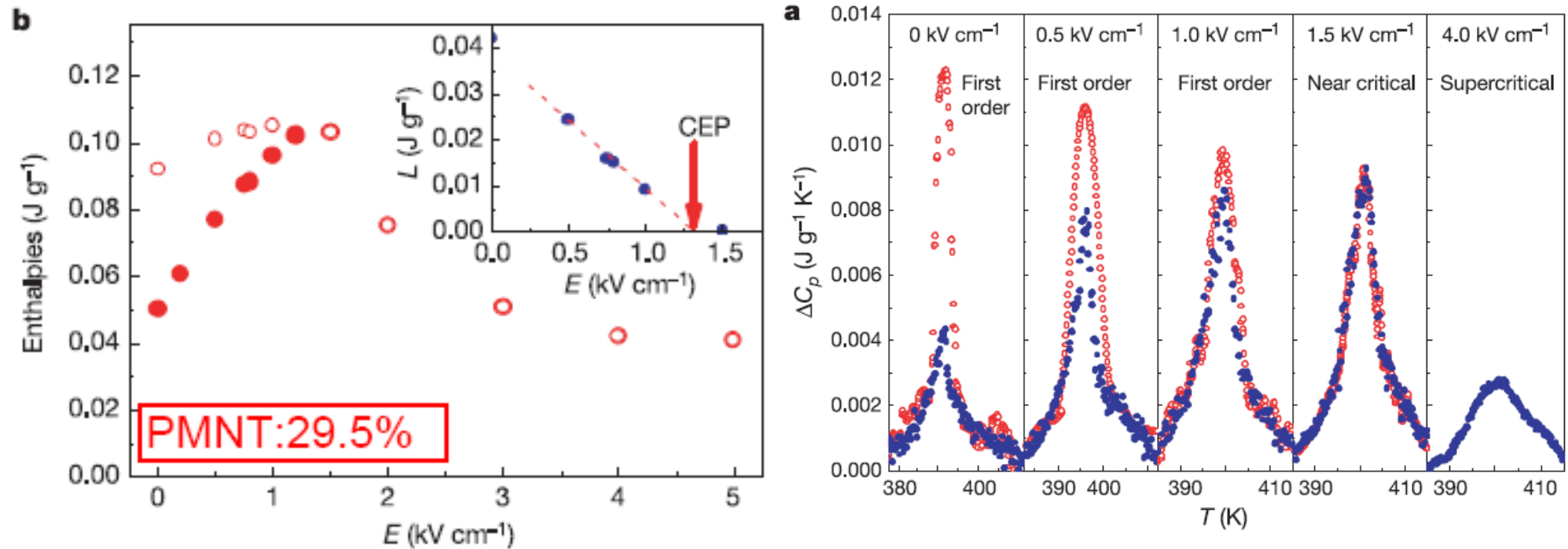
Results & discussion:

**Critical phenomena in relaxors
and enhanced piezoelectricity**



Results & discussion: enhanced piezoelectricity

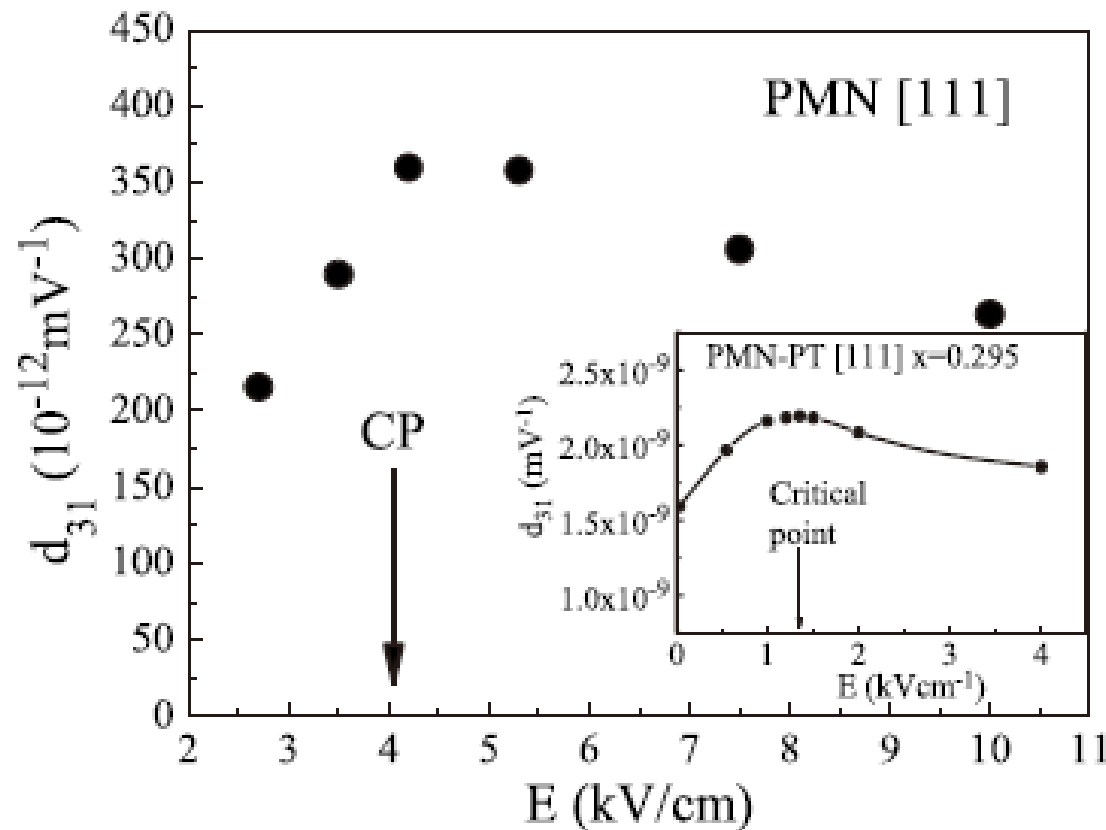
Critical phenomena



Z. Kutnjak, J. Petzelt, and R. Blinc, *Nature* **441**, 956 (2006).

Results & discussion: enhanced piezoelectricity

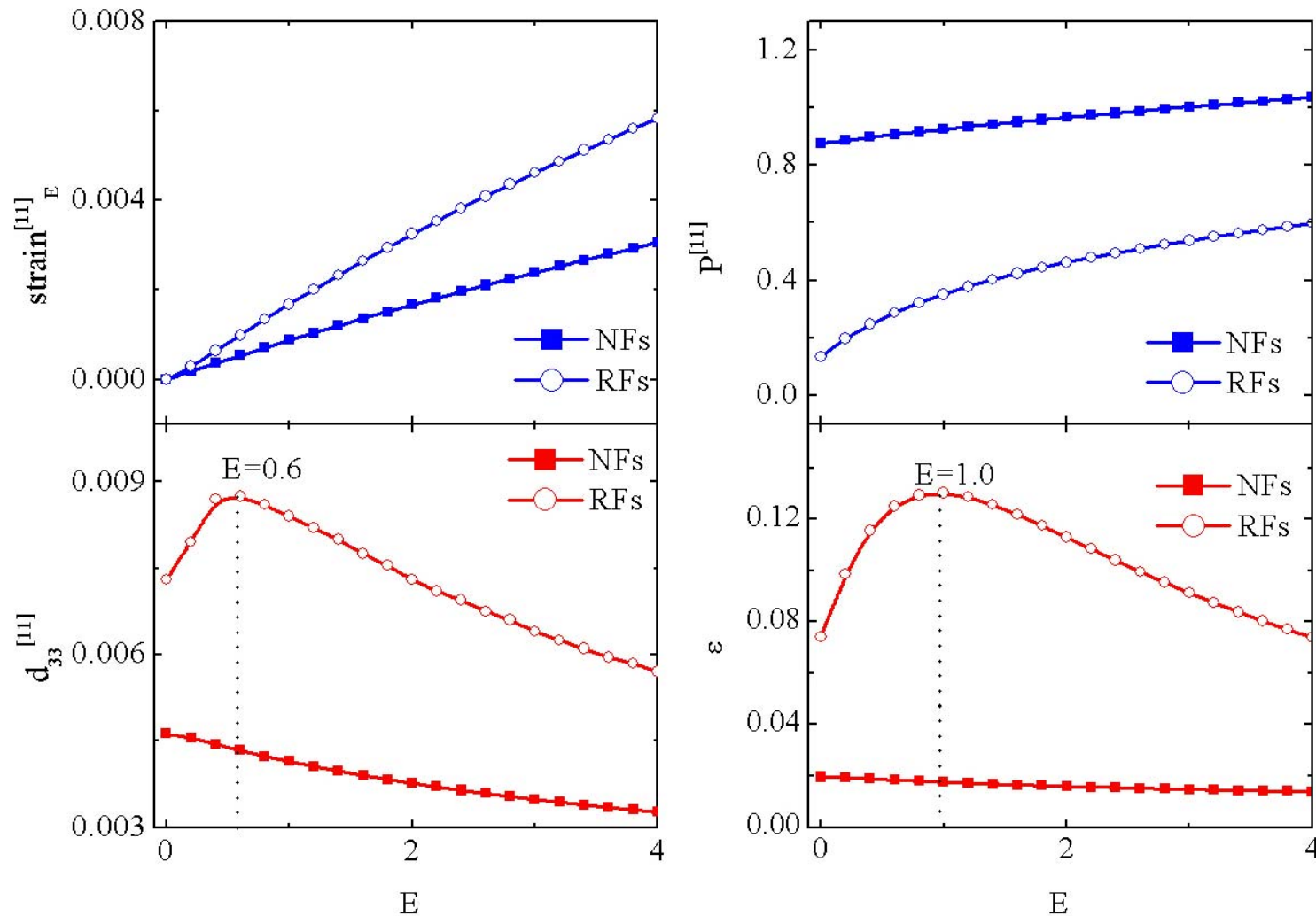
Critical phenomena



Z. Kutnjak, R. Blinc, and Y. Ishibashi, PRB **76**, 104102 (2007).

Results & discussion: enhanced piezoelectricity

Critical phenomena

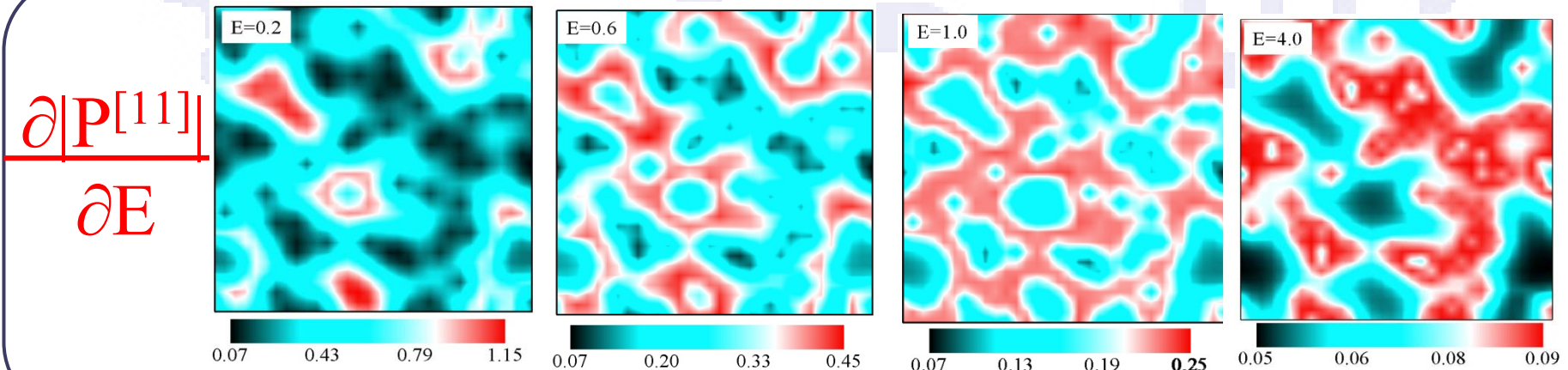
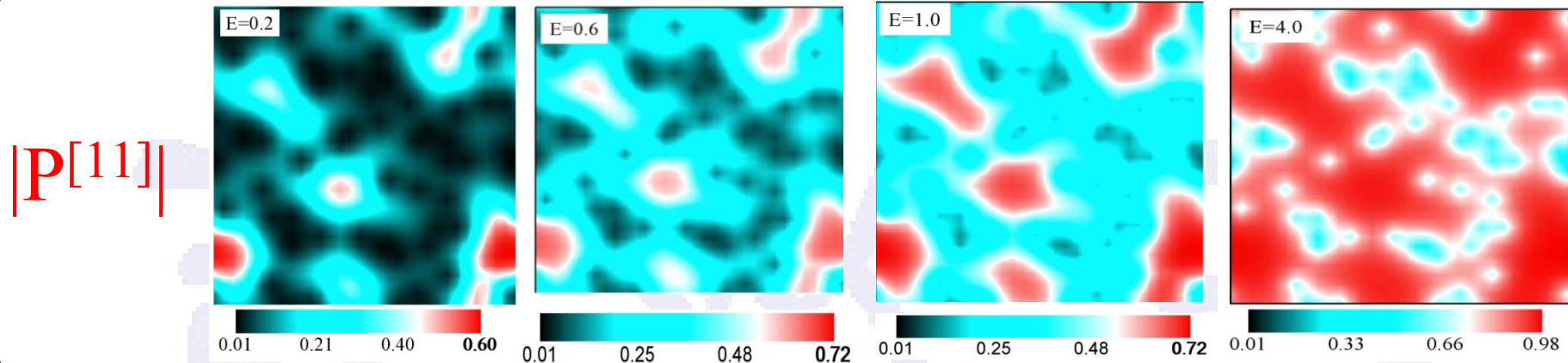


Poled $C_p=1.0$, $b_M=3.2$, $T=2.0$, $T_c=3.0$, $a=2$



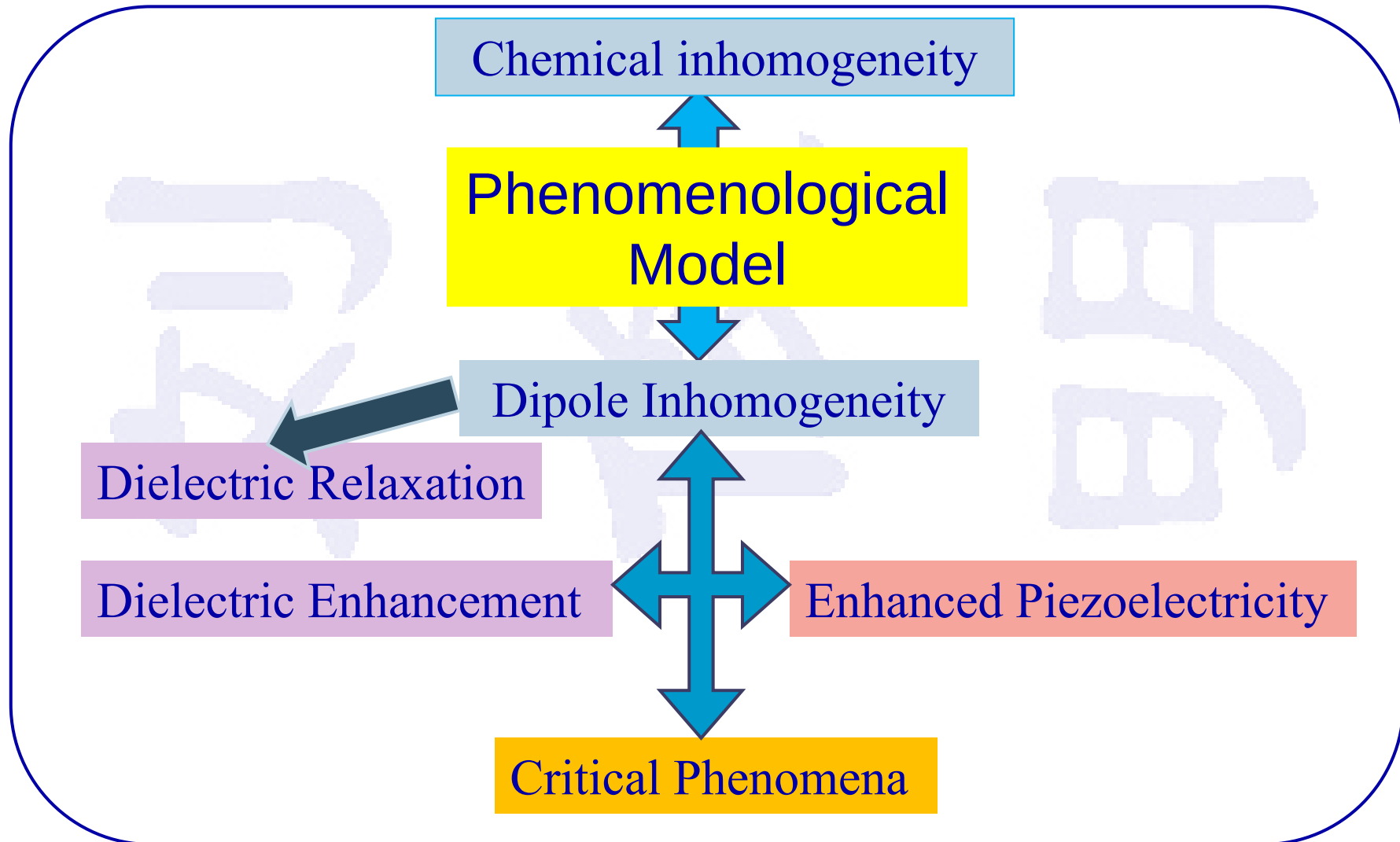
Results & discussion: enhanced piezoelectricity

Critical phenomena



Poled $C_p=1.0$, $b_M=3.2$, $T=2.0$, $T_c=3.0$, $a=2$

Summary



Acknowledgement

Tong Wei, Kai Xia, Ke-Feng Wang,
Shuai Dong, Chen Zhu, Chen-Liang Lu

National Natural Science Foundation of China
(Grant Nos. 10674061 and 50332020)

National Key Projects for Basic Research of
China No. (2002CB613303 and
2006CB921802)

Thank You



By ranma

