UNIVERSITY OF CAMBRIDGE

Electric polarisation in materials

Lecture 3

Bartomeu Monserrat
Course B: Materials for Devices

Professor M does Science

http://www.tcm.phy.cam.ac.uk/~bm418/

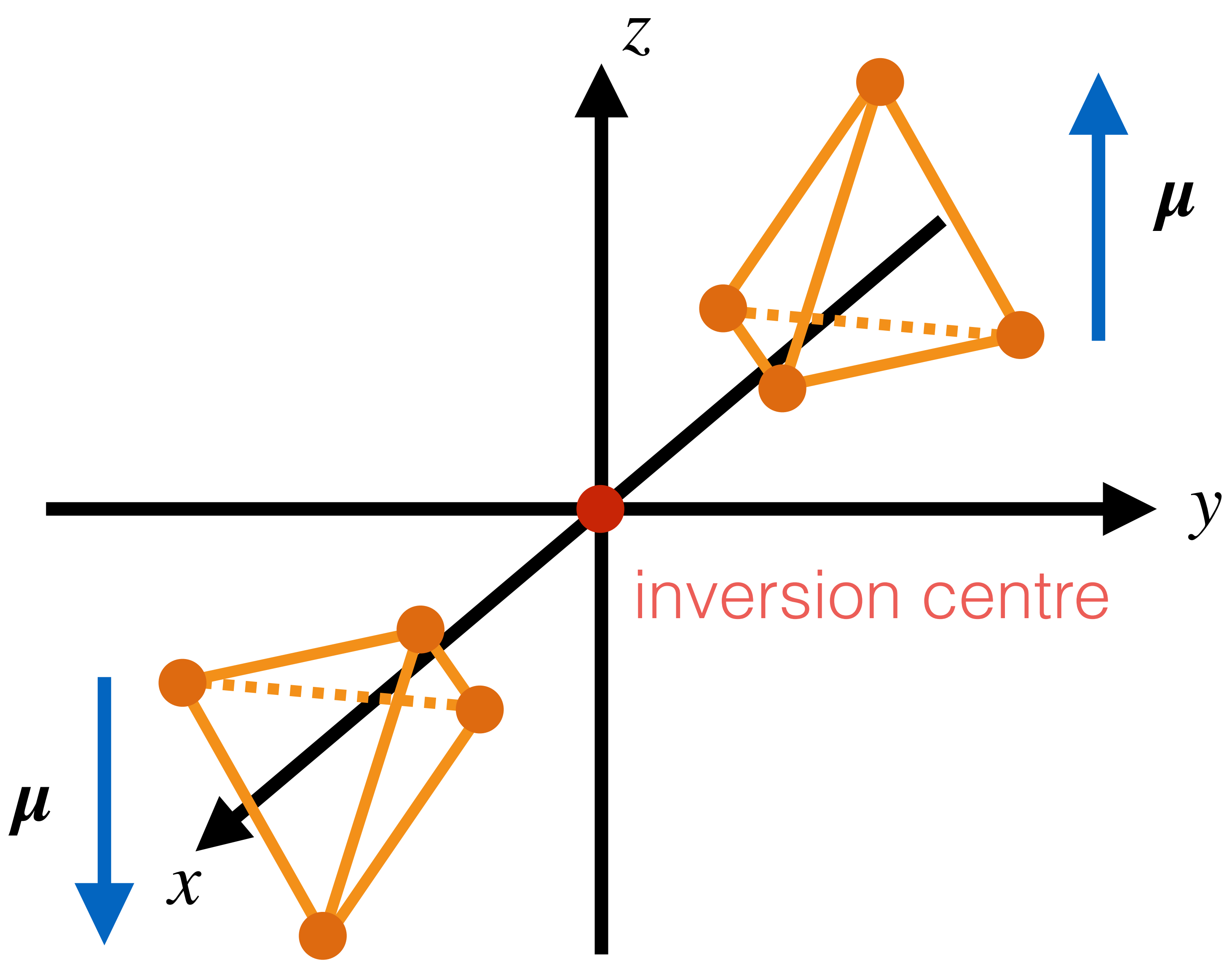
centrosymmetric crystal

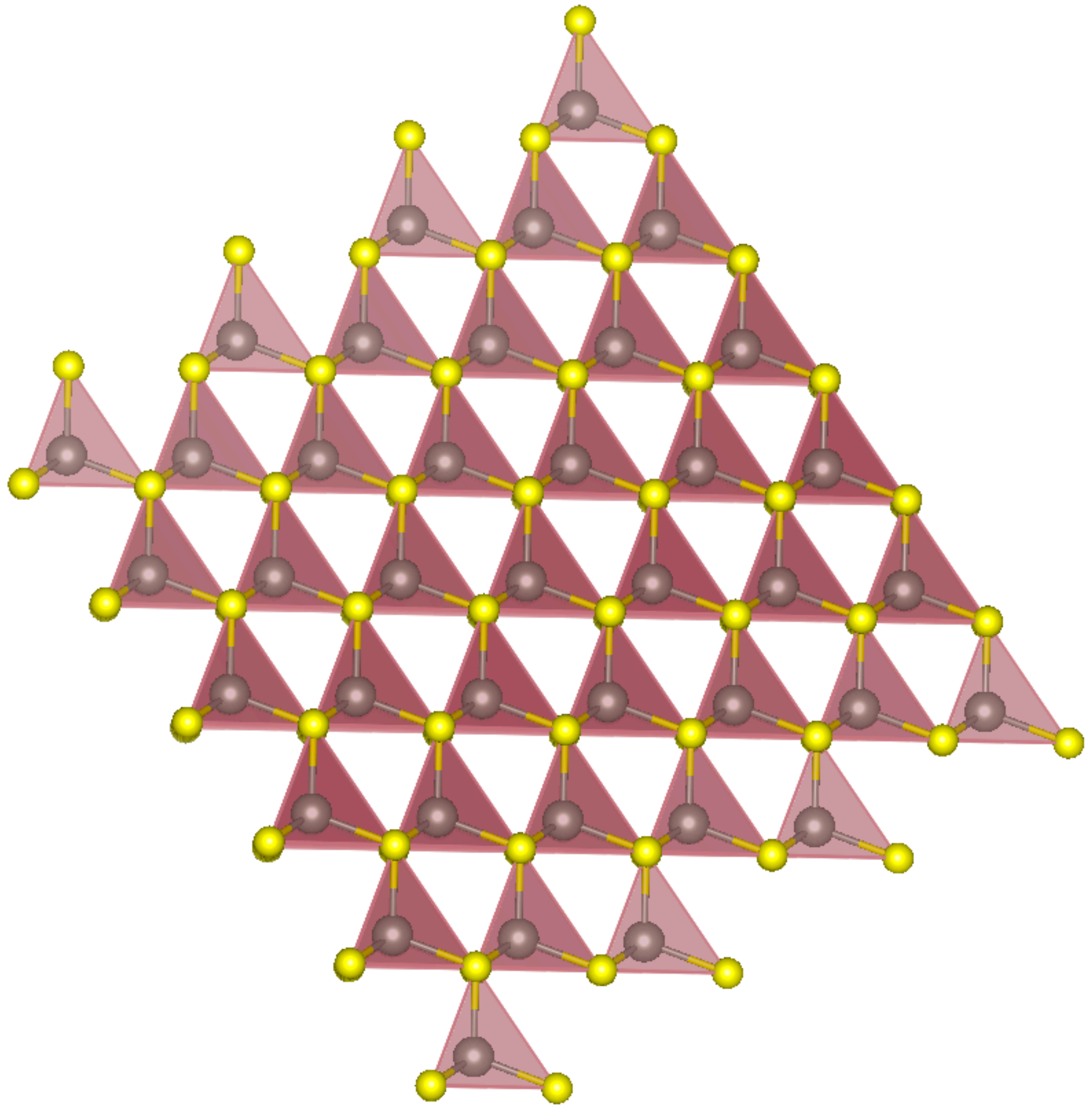
noncentrosymmetric crystal

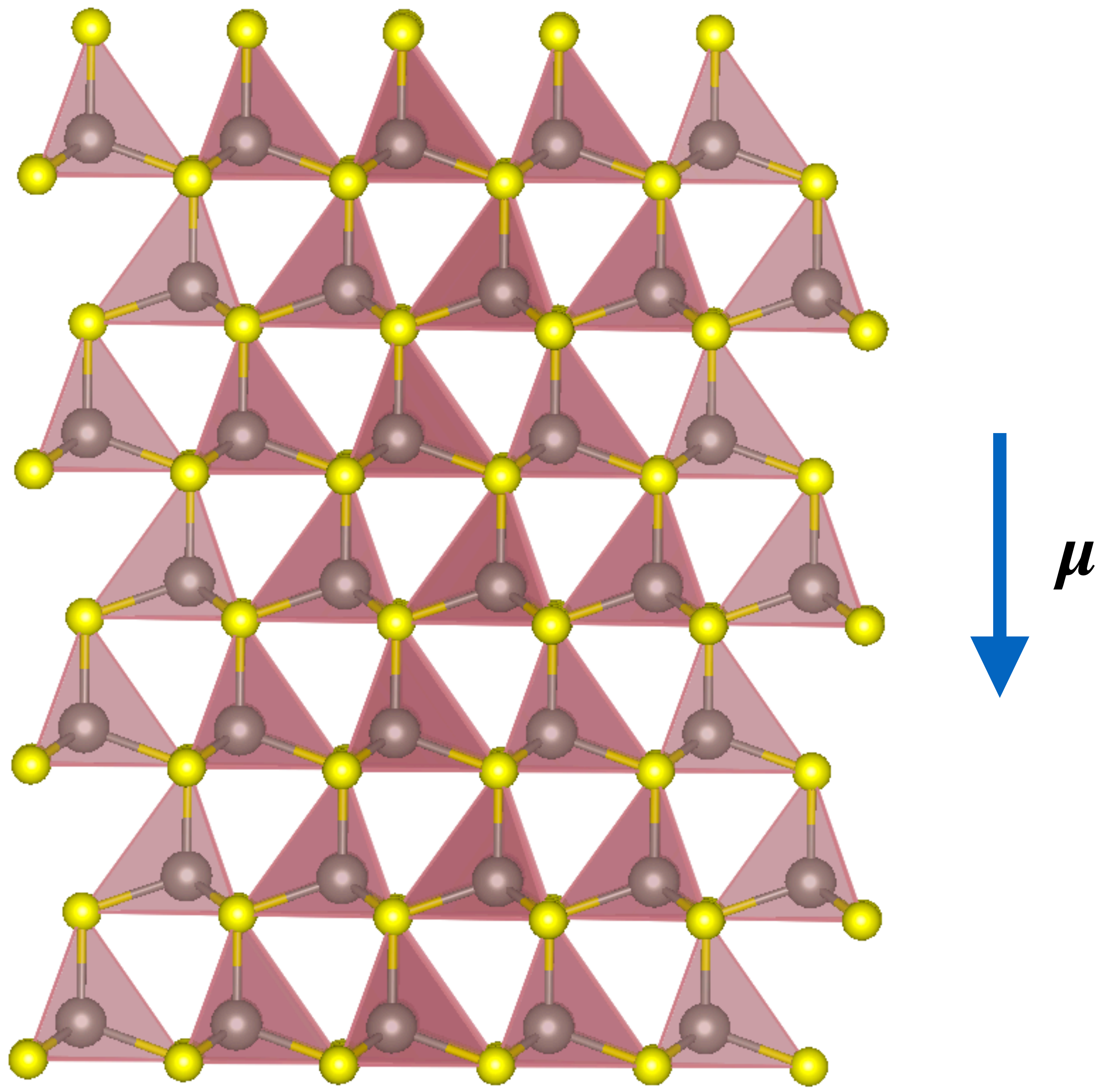
non-polar

non-polar

polar







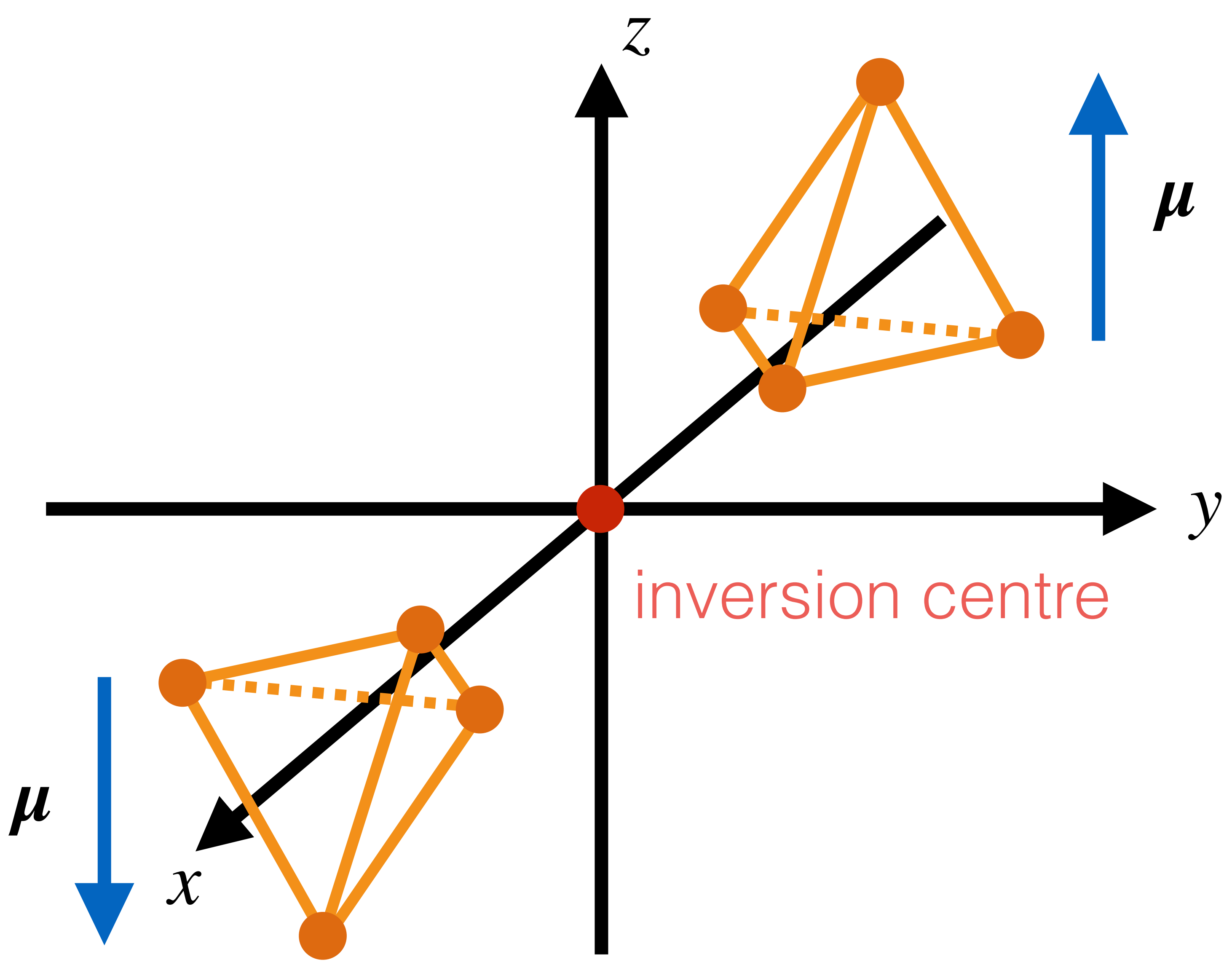
centrosymmetric crystal

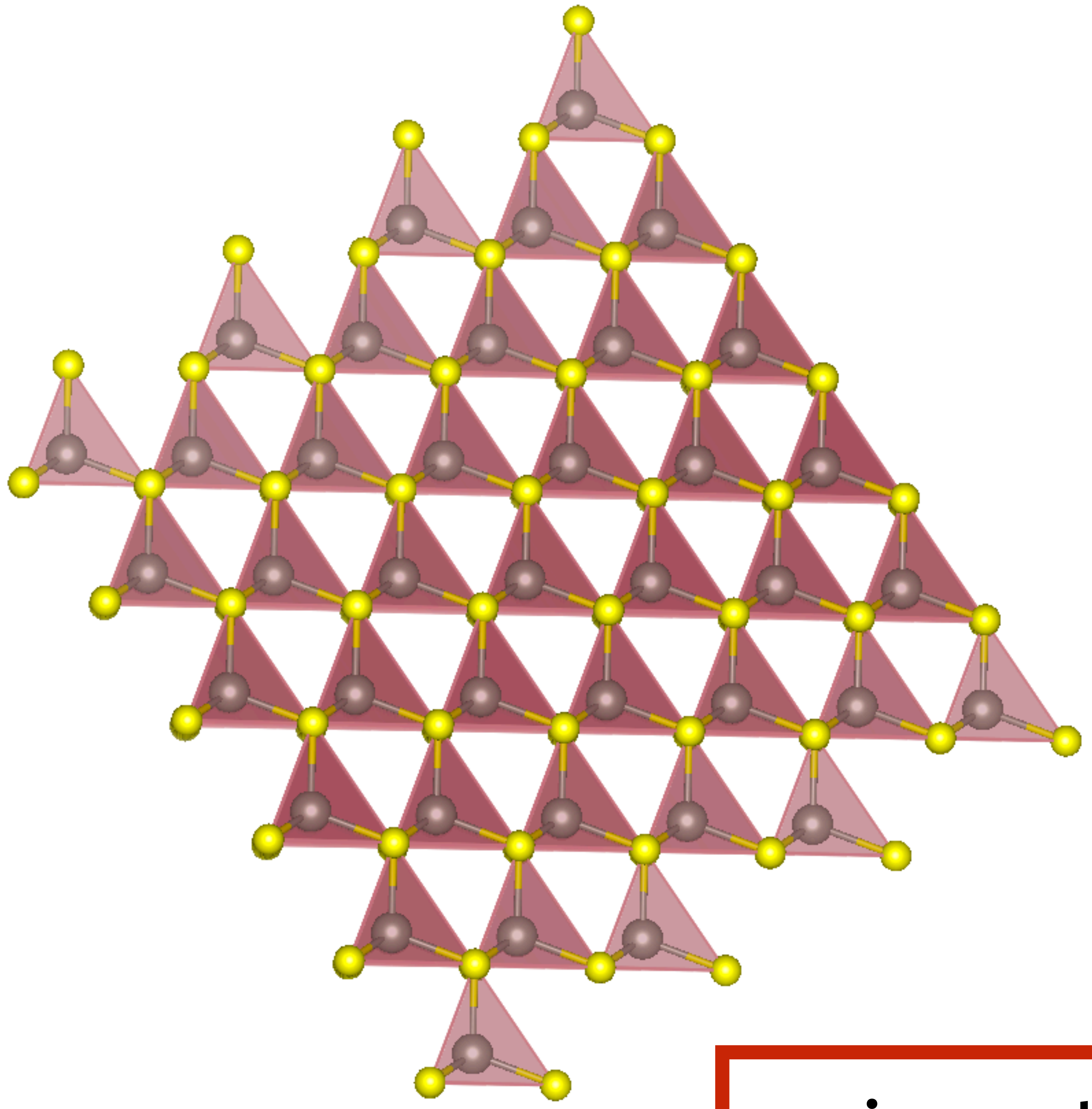
noncentrosymmetric crystal

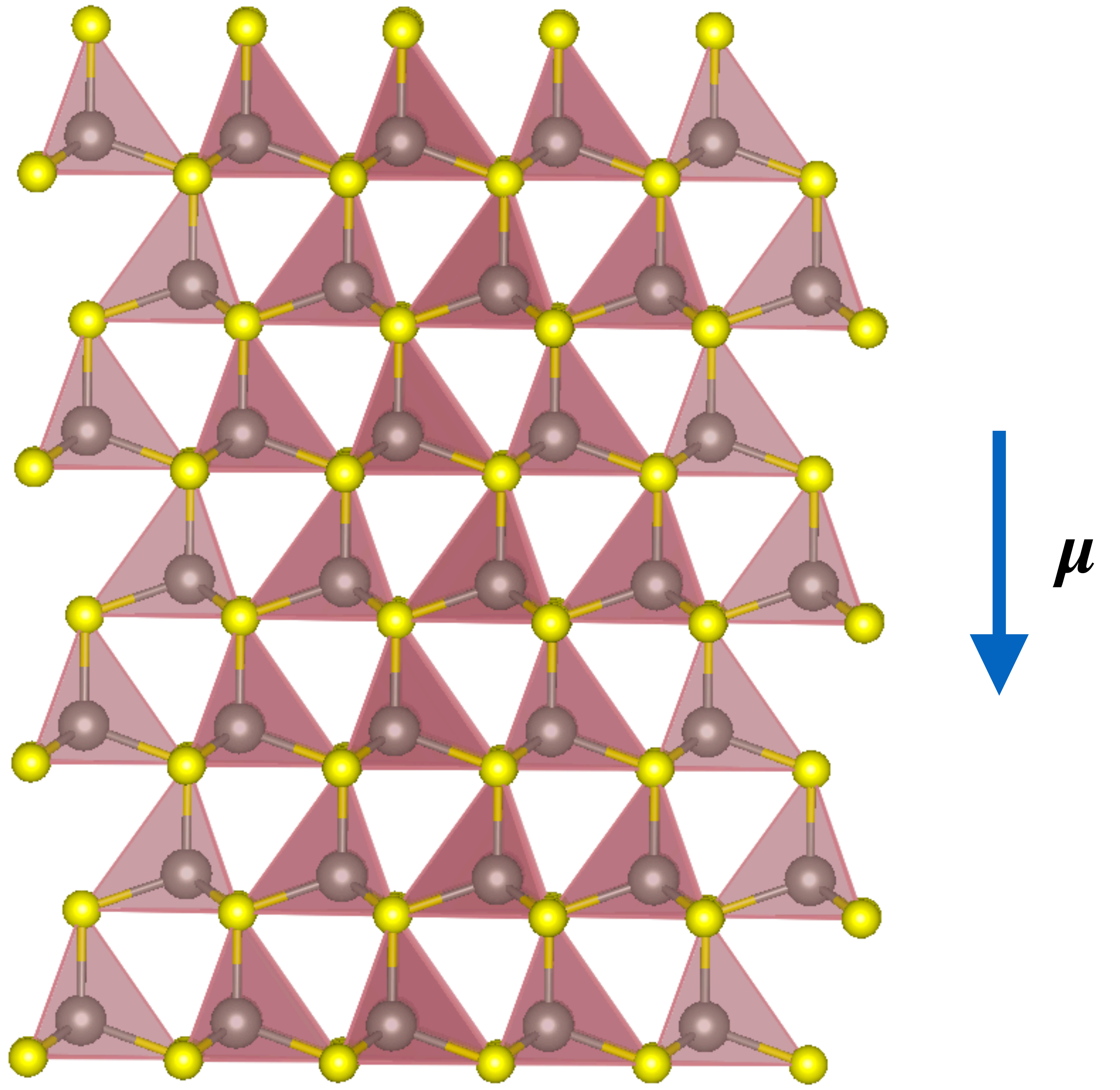
non-polar

non-polar

polar







no piezoelectricity

piezoelectricity*

* Cubic crystal class 432 exception

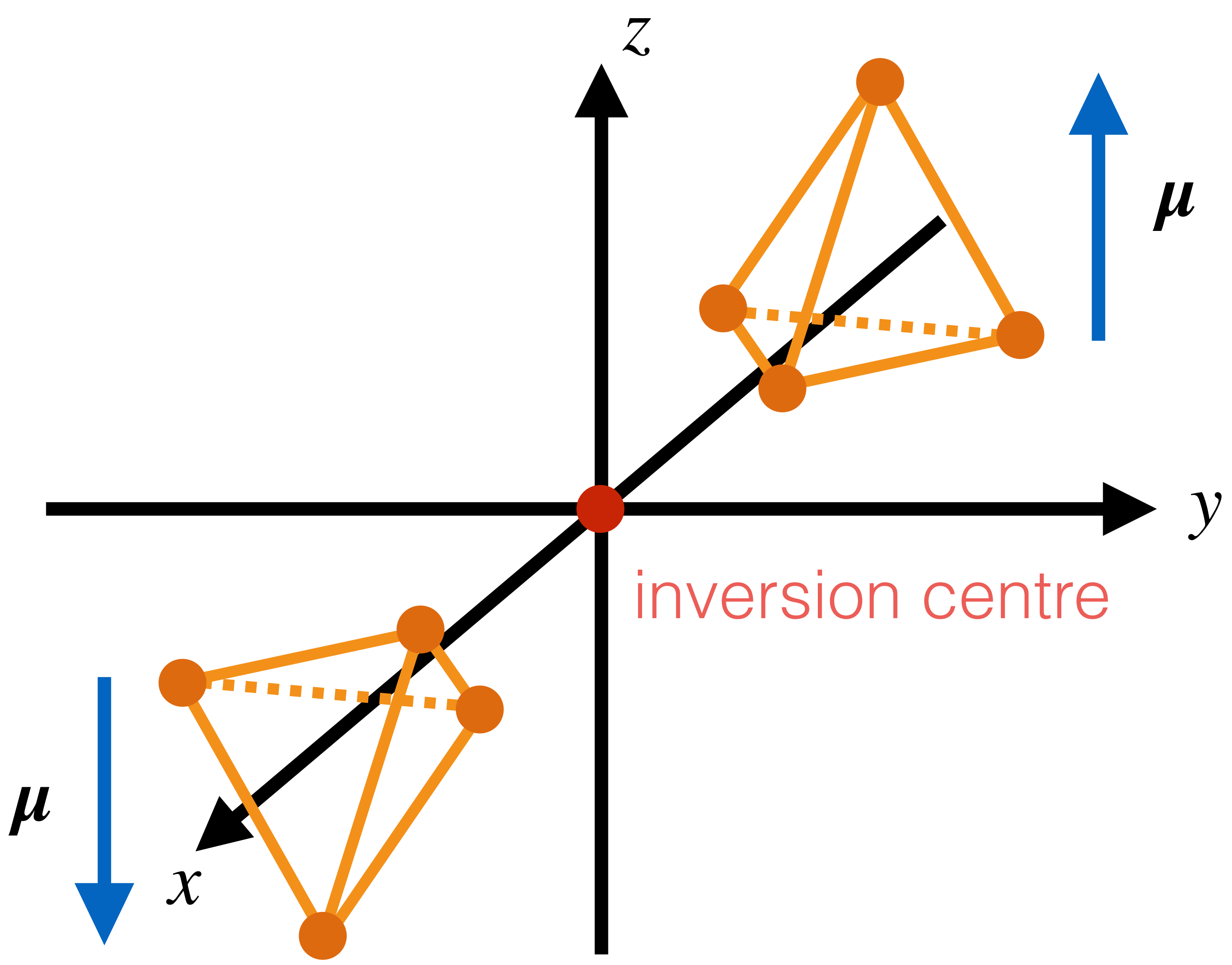
centrosymmetric crystal

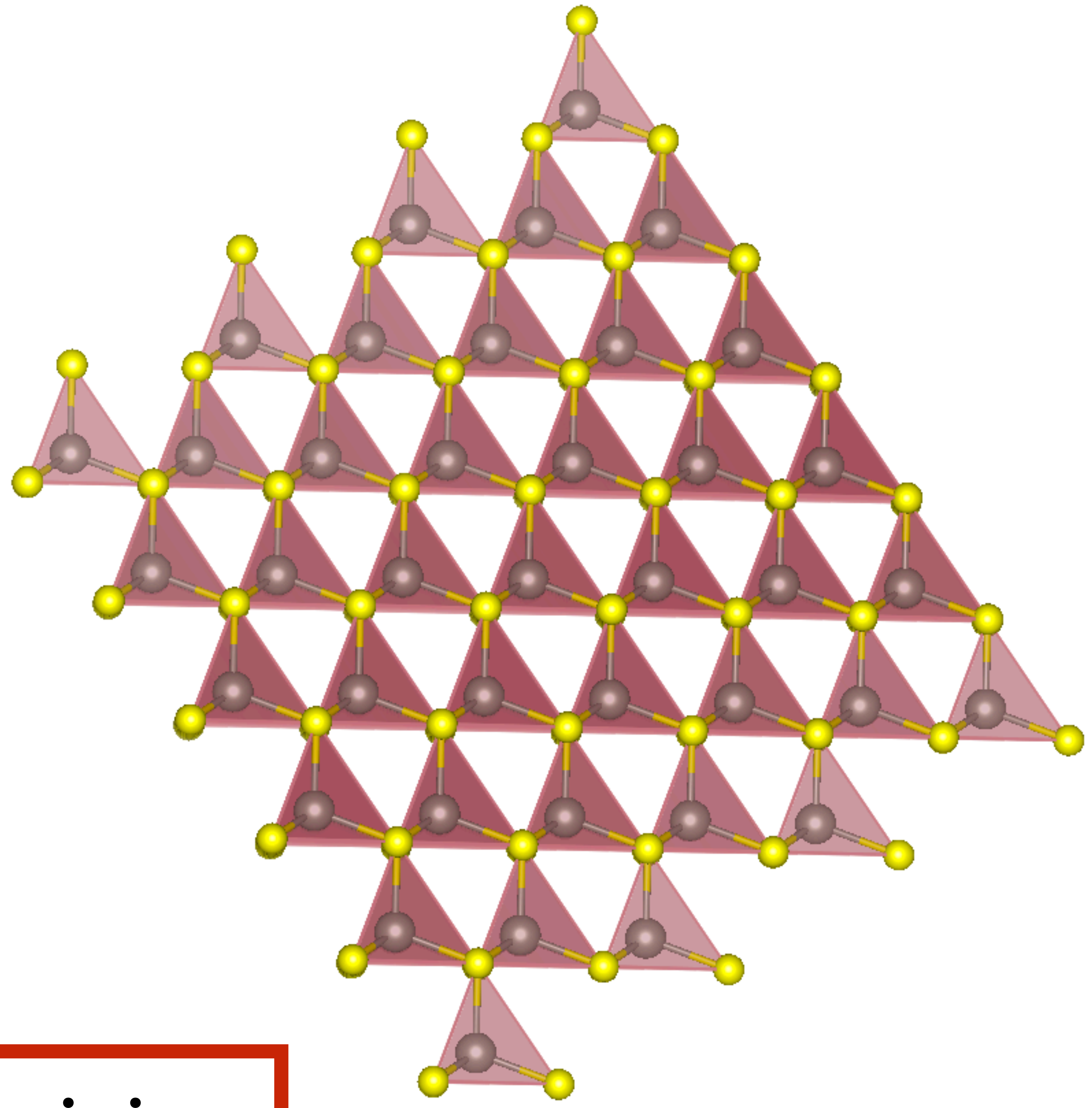
noncentrosymmetric crystal

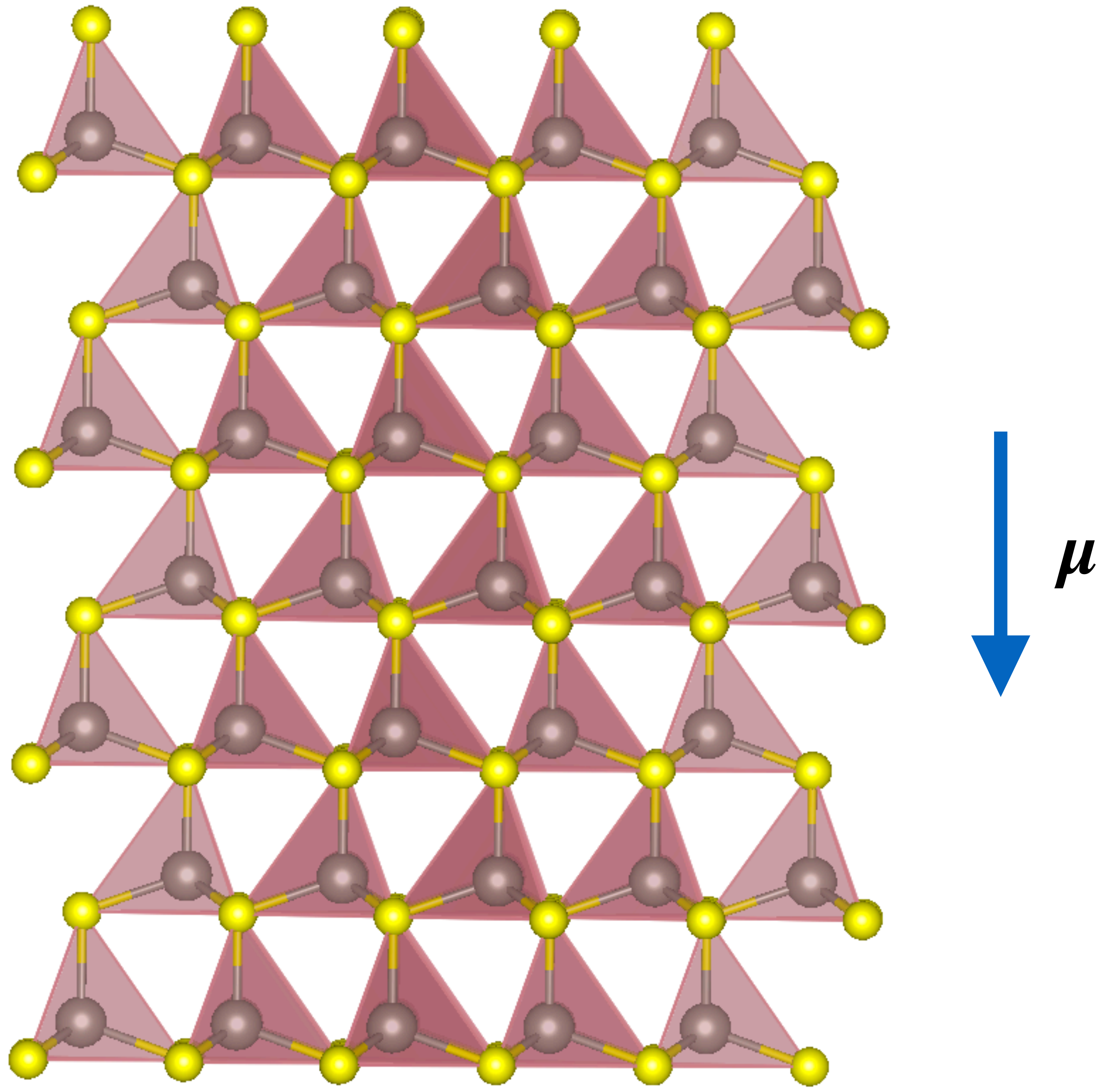
non-polar

non-polar

polar

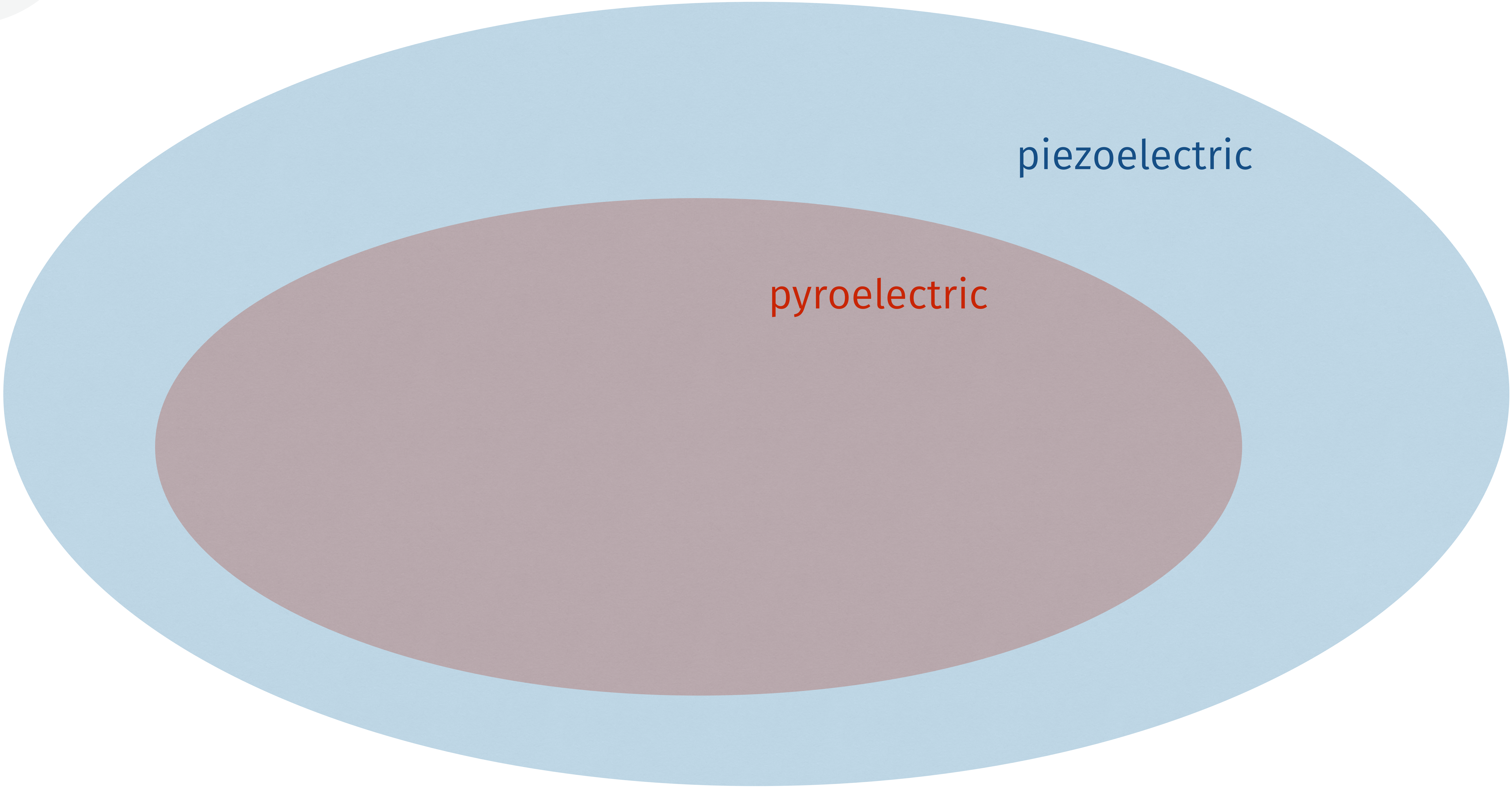


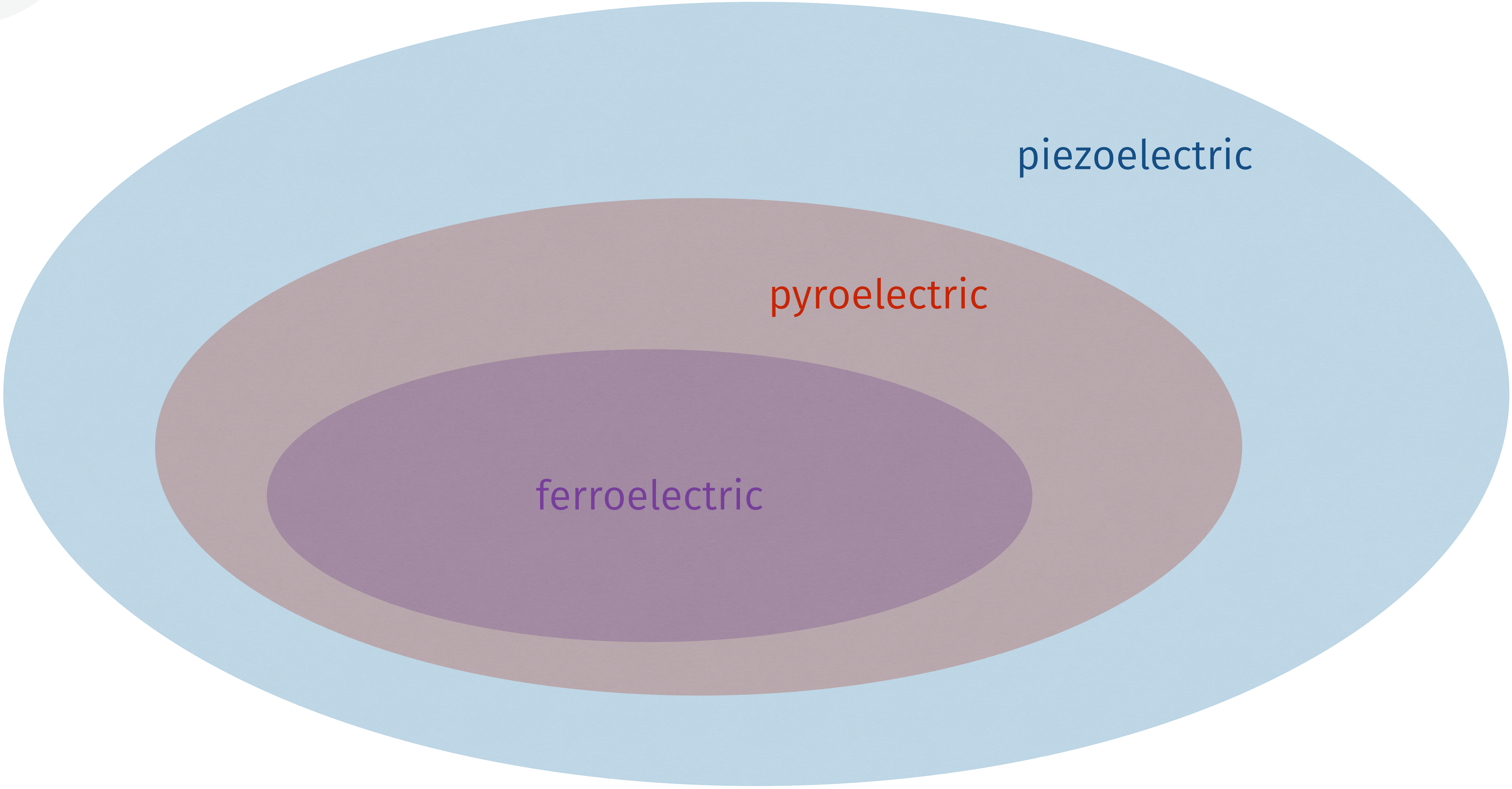




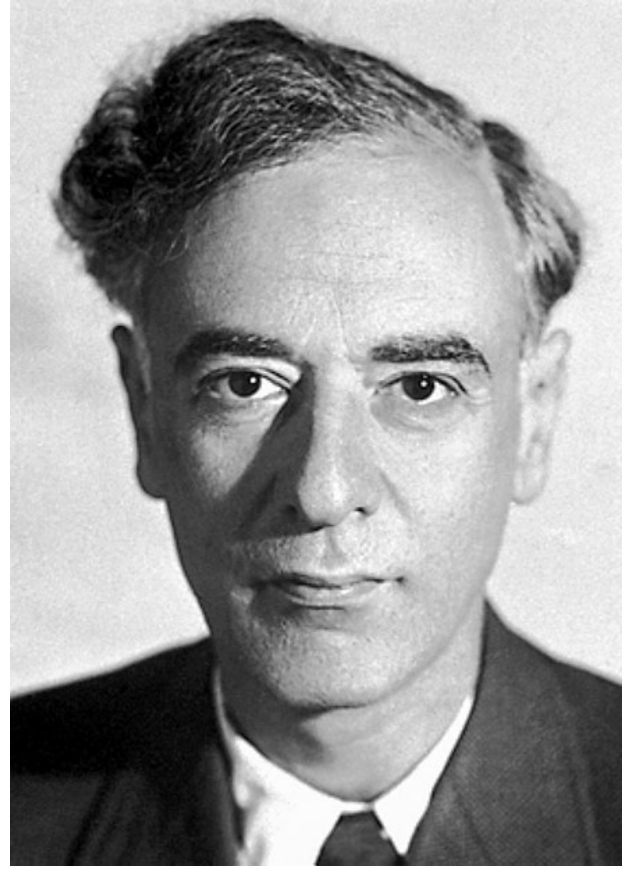
no pyroelectricity

pyroelectricity


piezoelectric
pyroelectric


piezoelectric
pyroelectric
ferroelectric

Landau theory



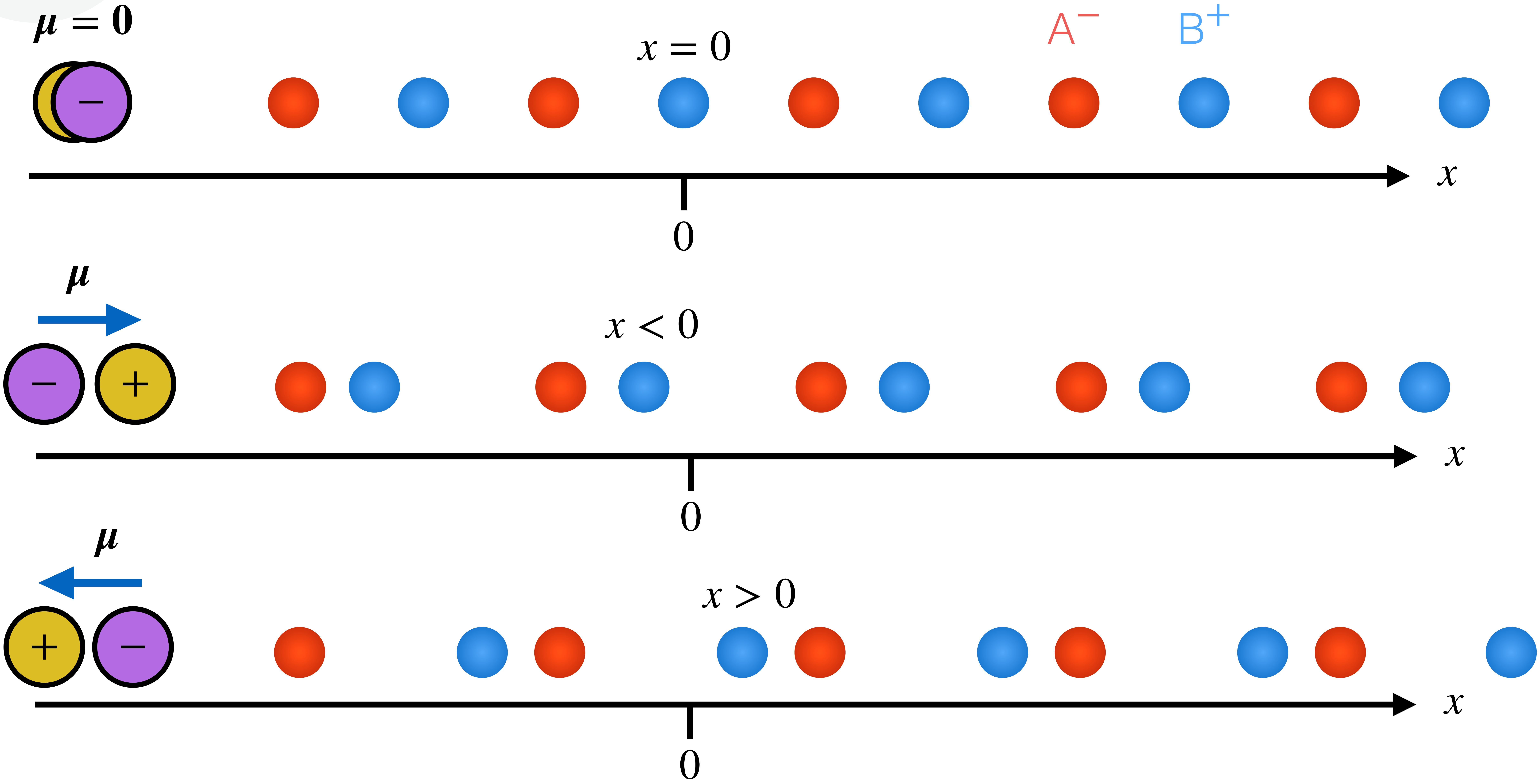
$$\mathscr{F}(P,T) = a(T - T_c)P^2 + \frac{b}{2}P^4 - EP$$

Lev Landau

Nobel Prize in Physics 1962

"for pioneering theories for condensed matter, especially liquid helium"

Landau theory

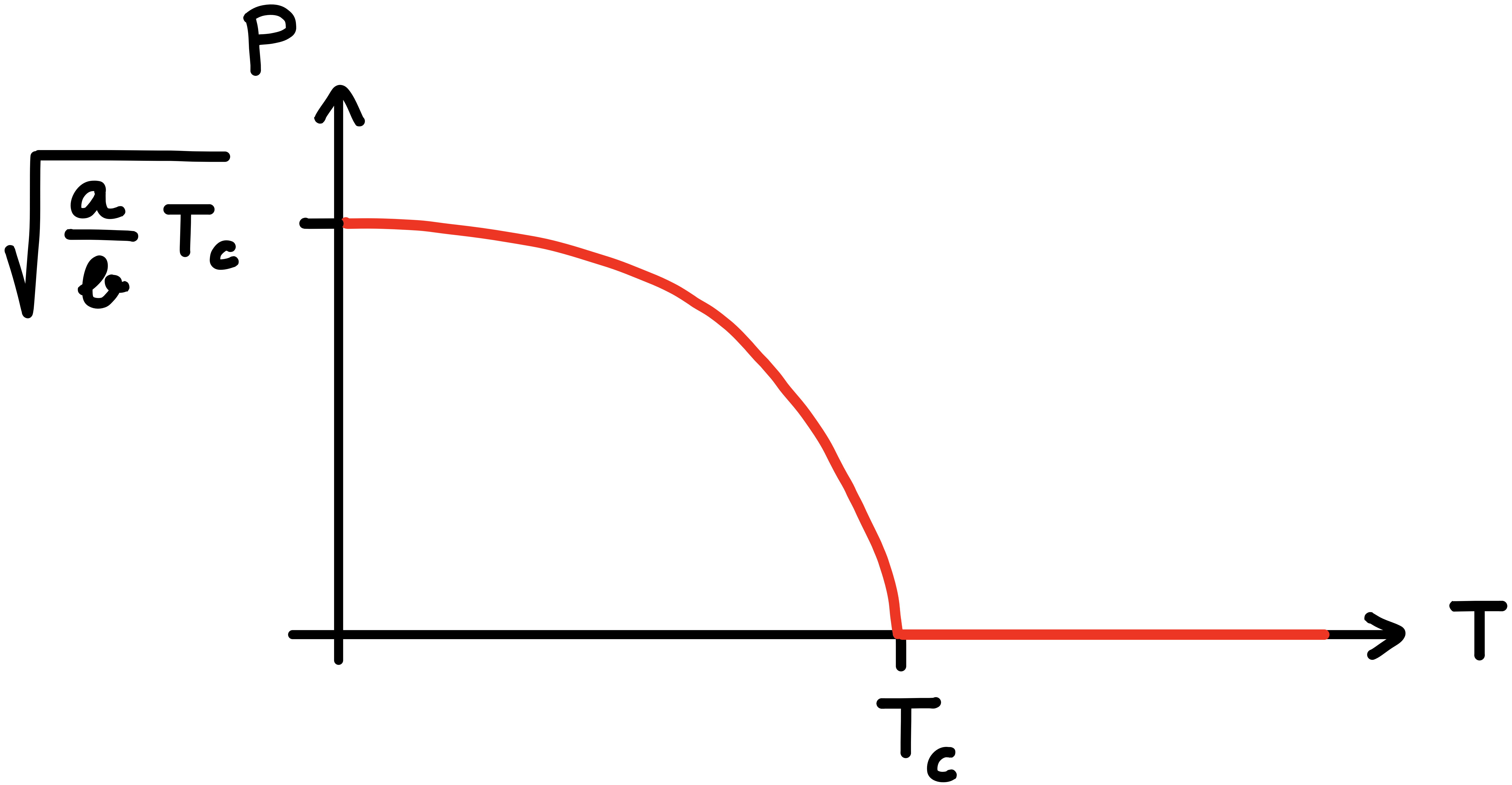


Landau theory

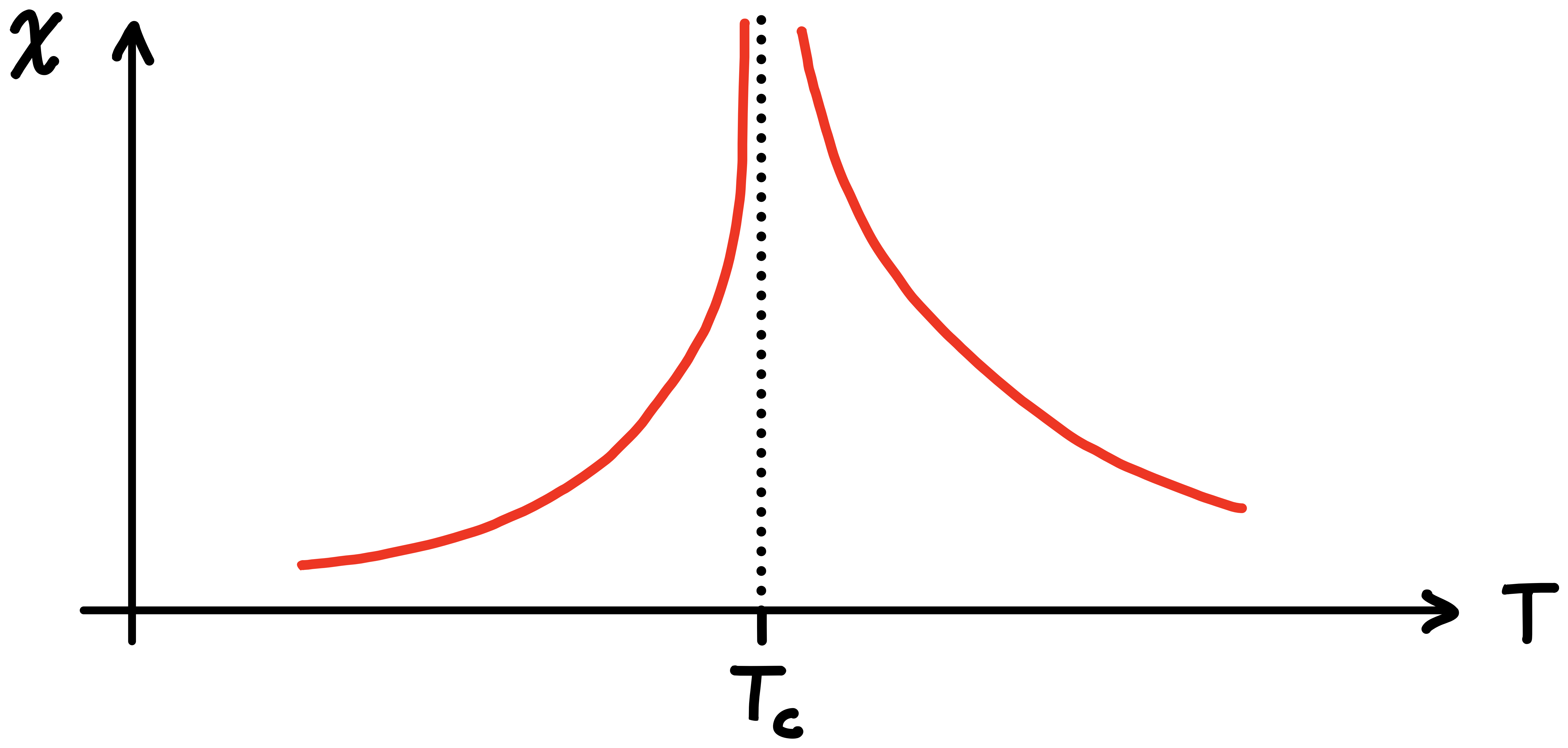
- *See discussion of Landau theory*

$$\mathcal{F}(P, T) = a(T - T_c)P^2 + \frac{b}{2}P^4 - EP$$

Landau theory



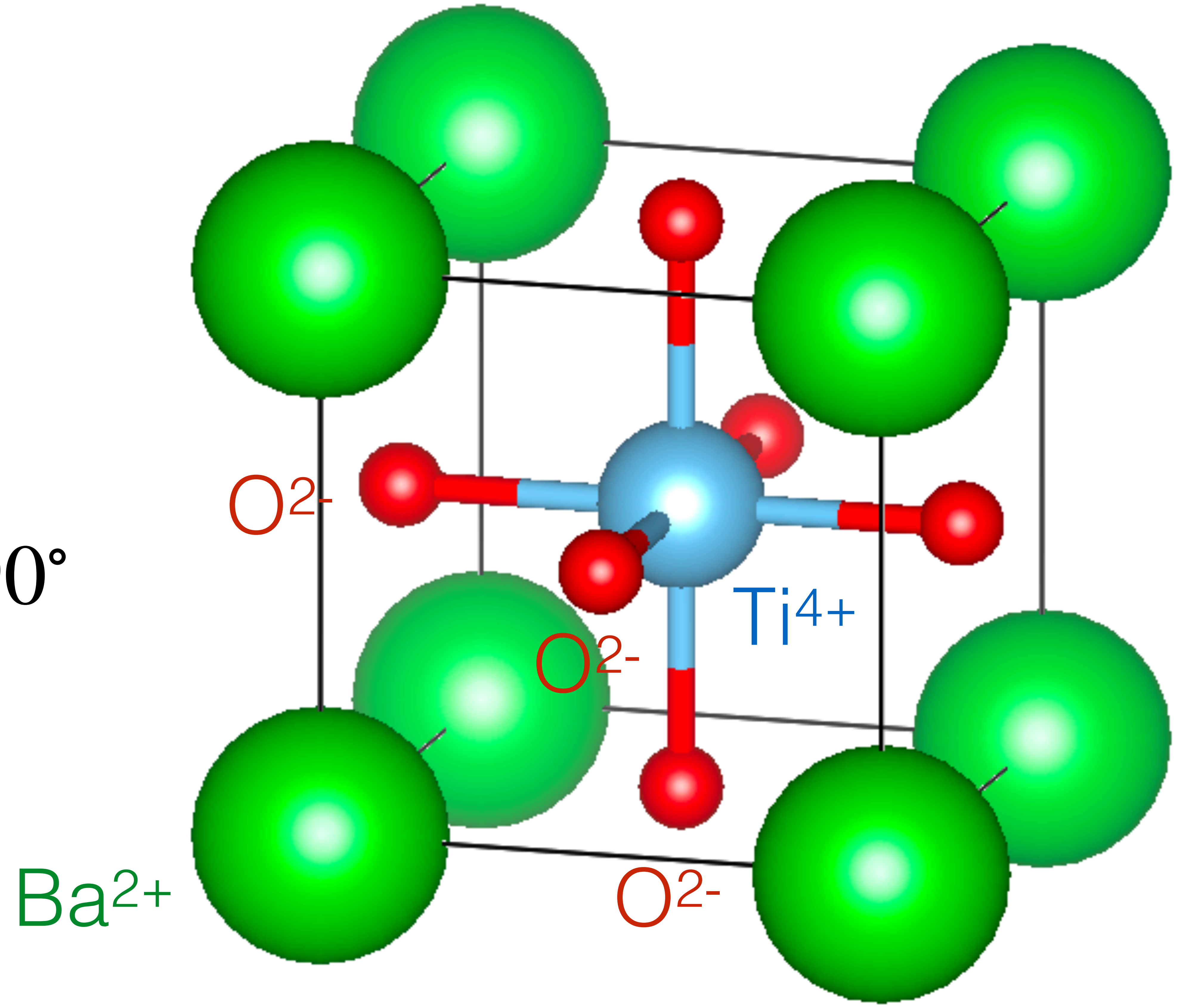
Landau theory



Perovskite structure ABX_3

$$a = b = c$$

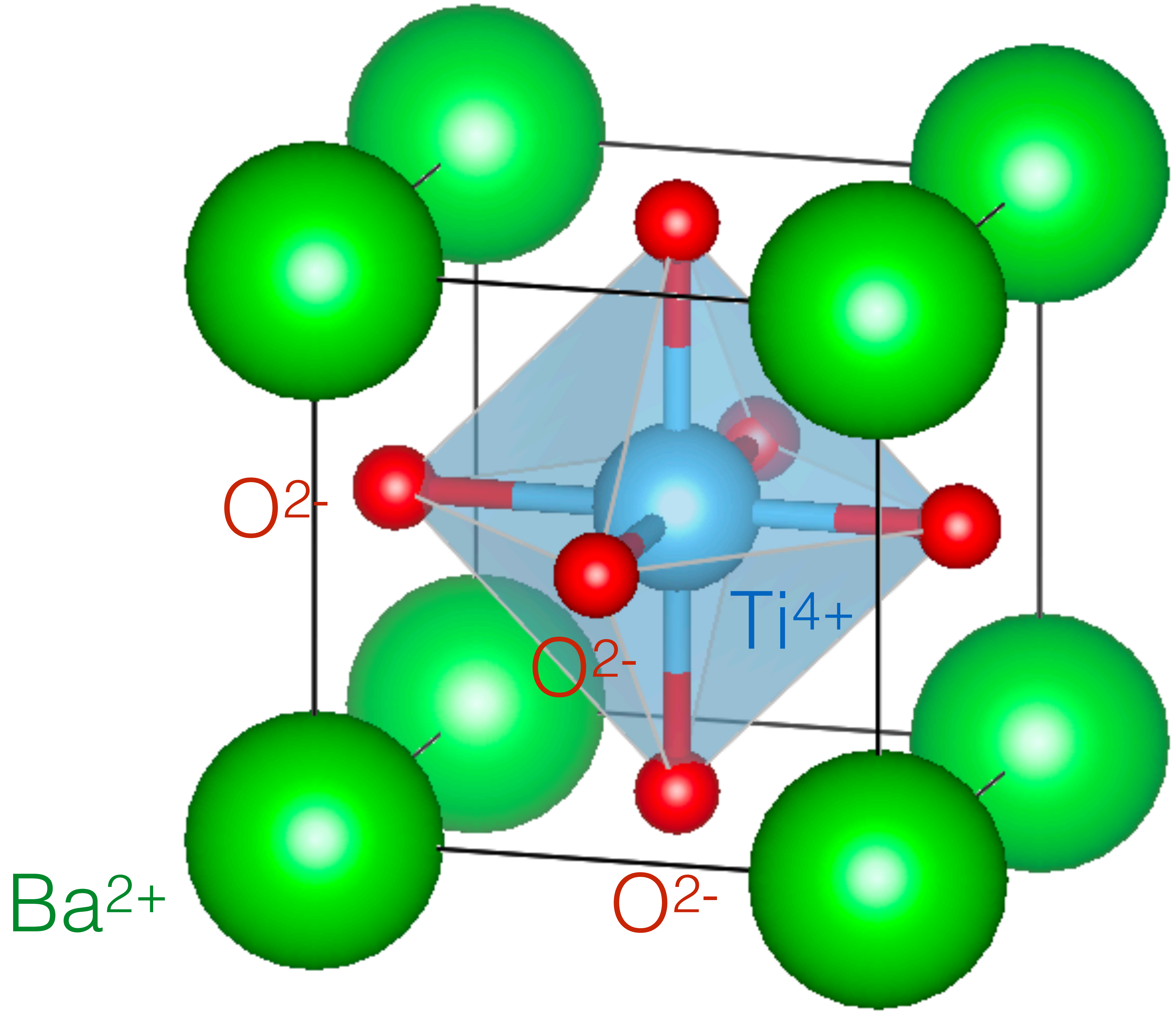
$$\alpha = \beta = \gamma = 90°$$



- $BaTiO_3$
- Cubic
- Five-atom basis
- Centrosymmetric
- Course A

- *See structure model in 3D*

Perovskite structure ABX_3



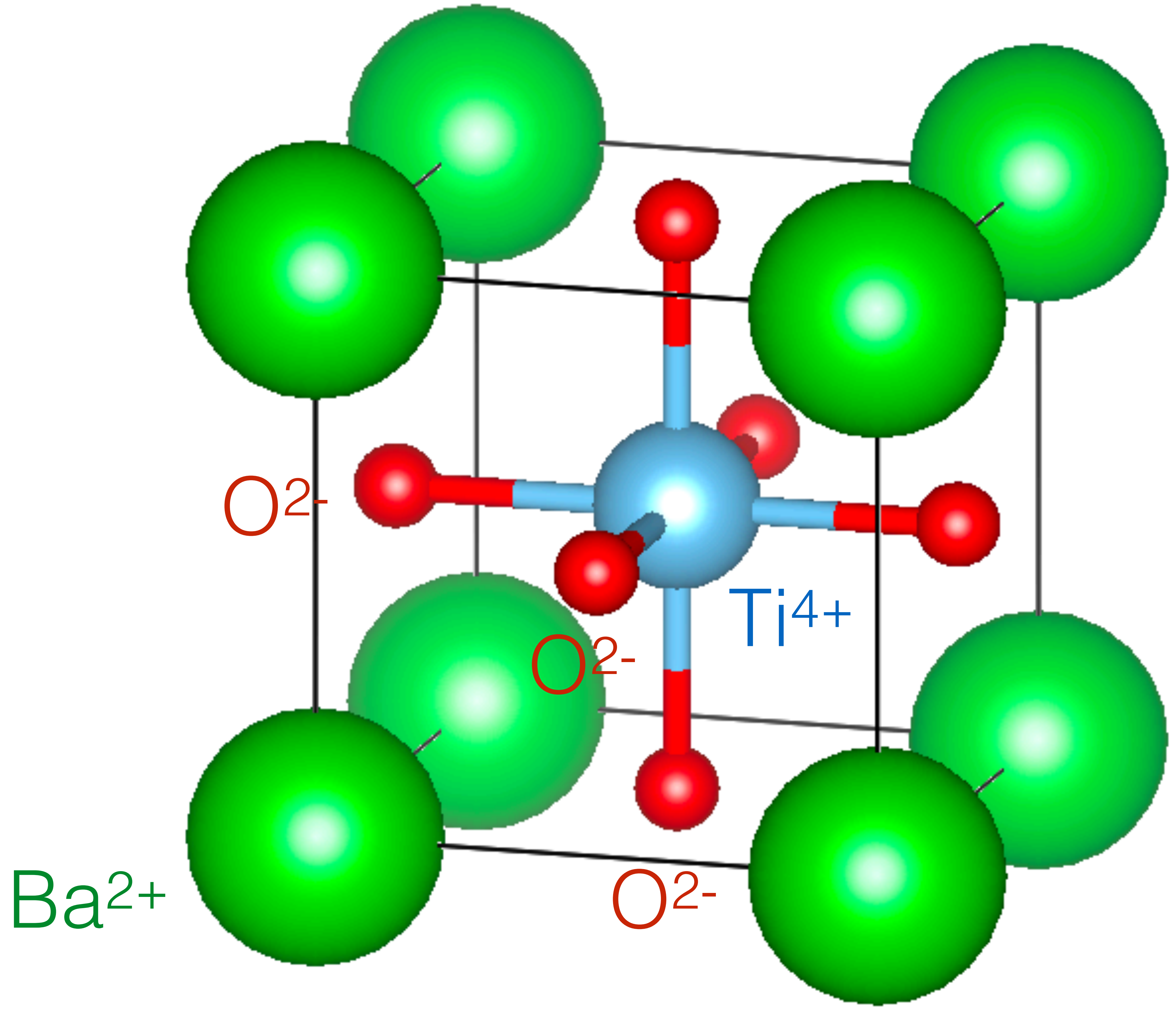
- $BaTiO_3$
- Cubic
- Five-atom basis
- Centrosymmetric
- Course A

Goldschmidt tolerance factor for ABX_3 perovskite

- *See Problem 3*

$$t = \frac{r_\mathrm{A} + r_\mathrm{X}}{\sqrt{2}(r_\mathrm{B} + r_\mathrm{X})}$$

Goldschmidt tolerance factor for $BaTiO_3$ perovskite



$$t = \frac{r_A + r_X}{\sqrt{2}(r_B + r_X)}$$

$$r_A = r_{Ba^{2+}} = 1.75\ \text{Å}$$

$$r_B = r_{Ti^{4+}} = 0.75\ \text{Å}$$

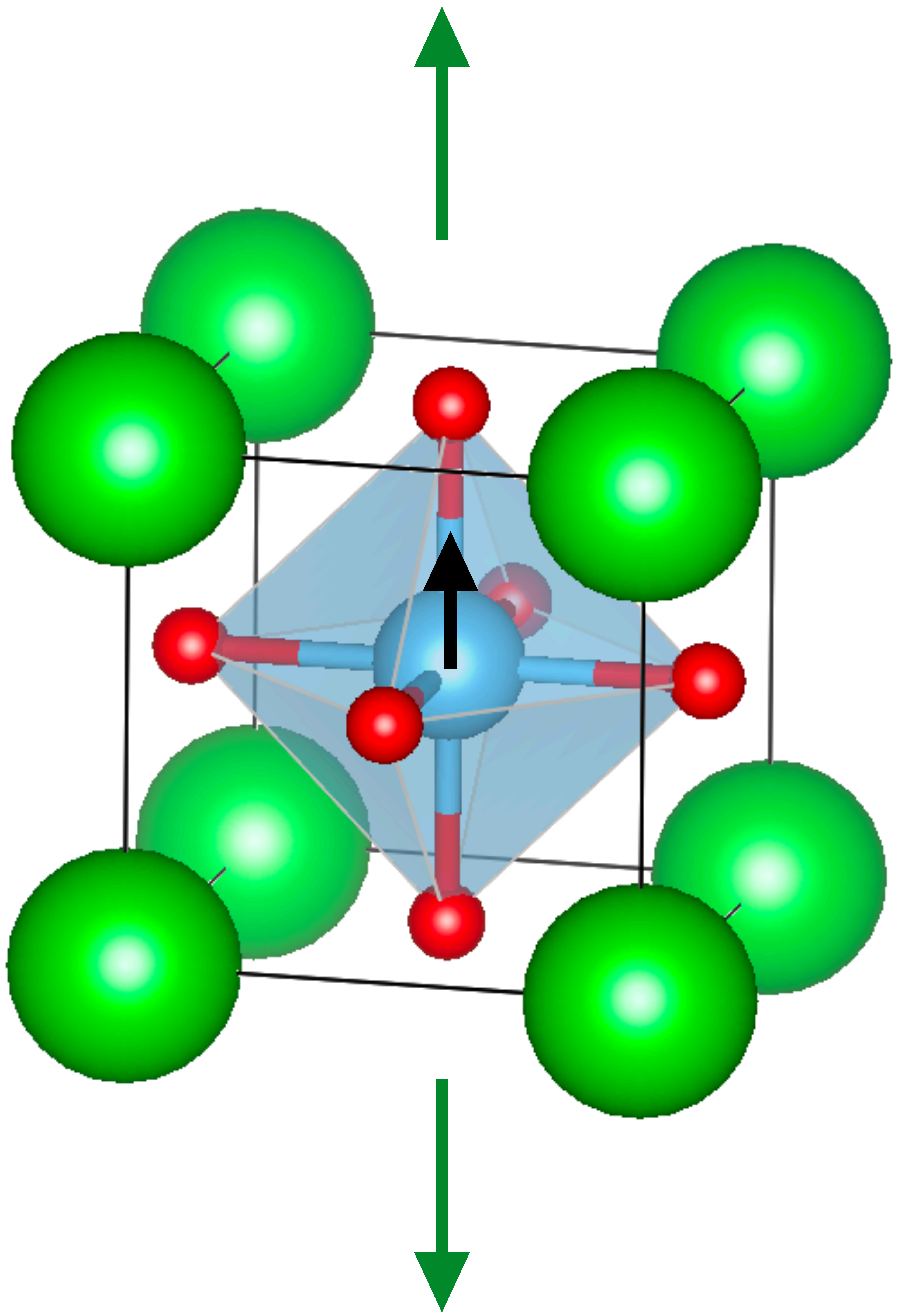
$$r_X = r_{O^{2-}} = 1.21\ \text{Å}$$

$$t = \frac{r_{Ba^{2+}} + r_{O^{2-}}}{\sqrt{2}(r_{Ti^{4+}} + r_{O^{2-}})} \simeq 1.07$$

Perovskite structure ABO_3

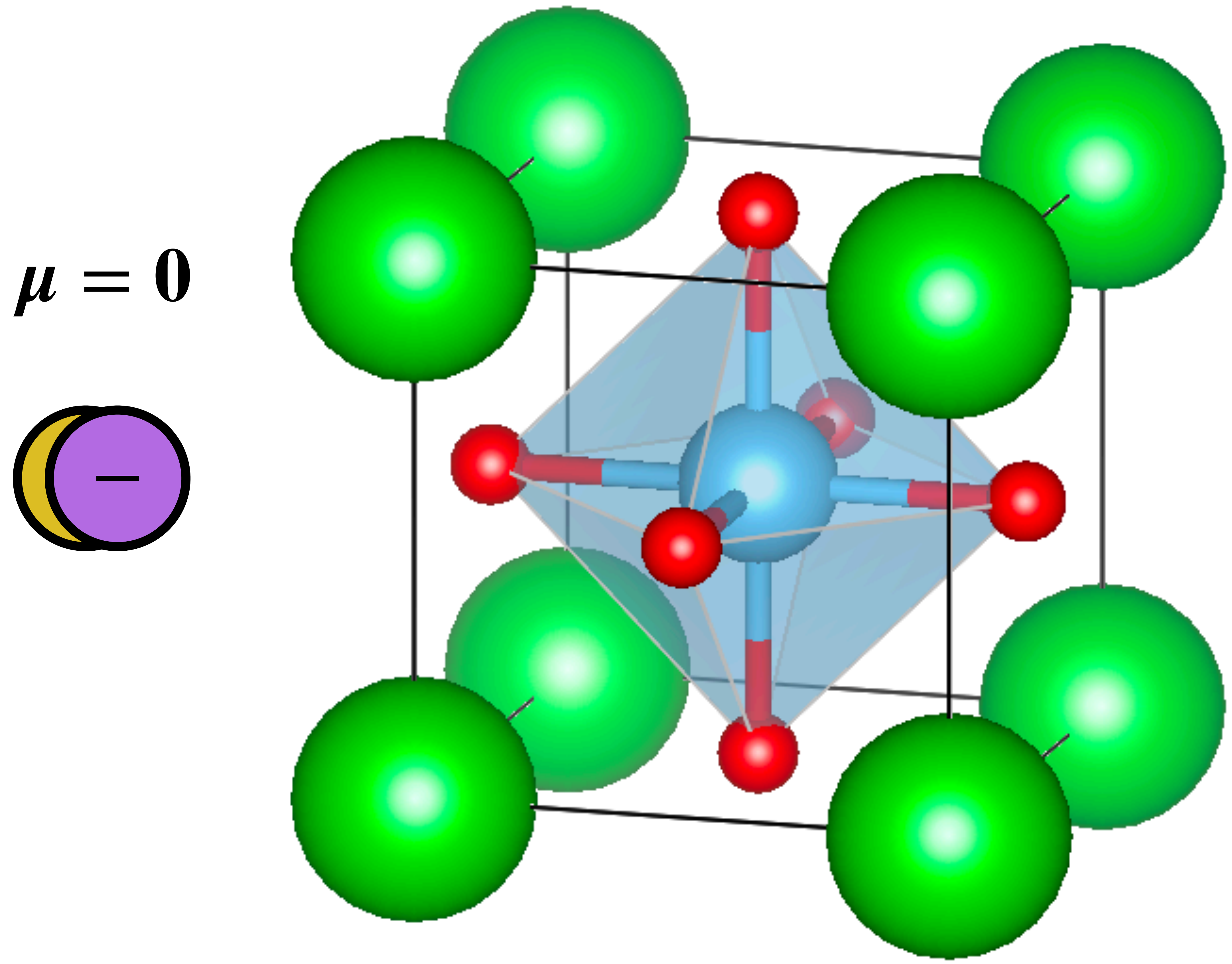
$$a = b < c$$

$$\alpha = \beta = \gamma = 90^\circ$$

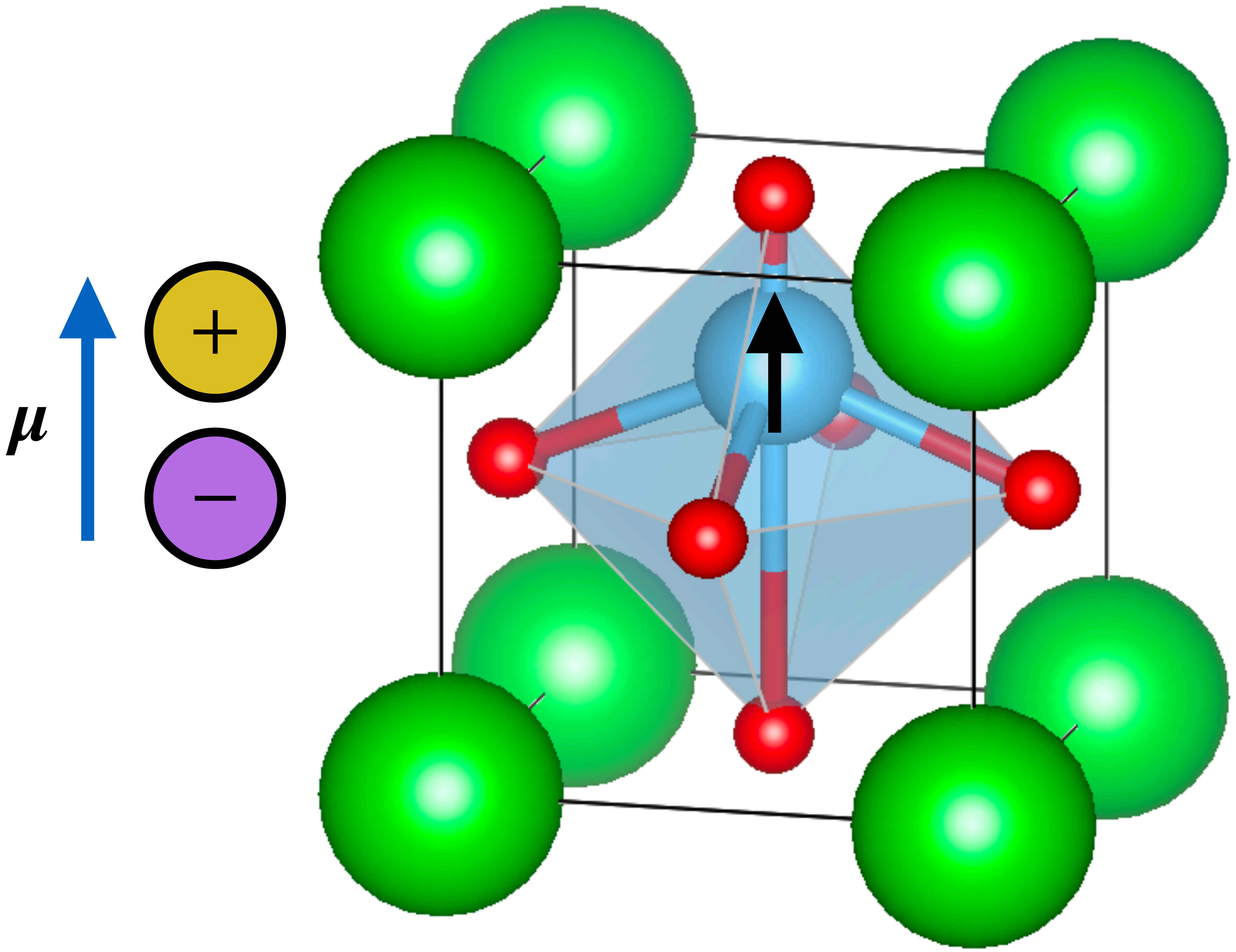


- $BaTiO_3$
- Tetragonal
- Five-atom basis
- Non-centrosymmetric

Perovskite structure ABO_3

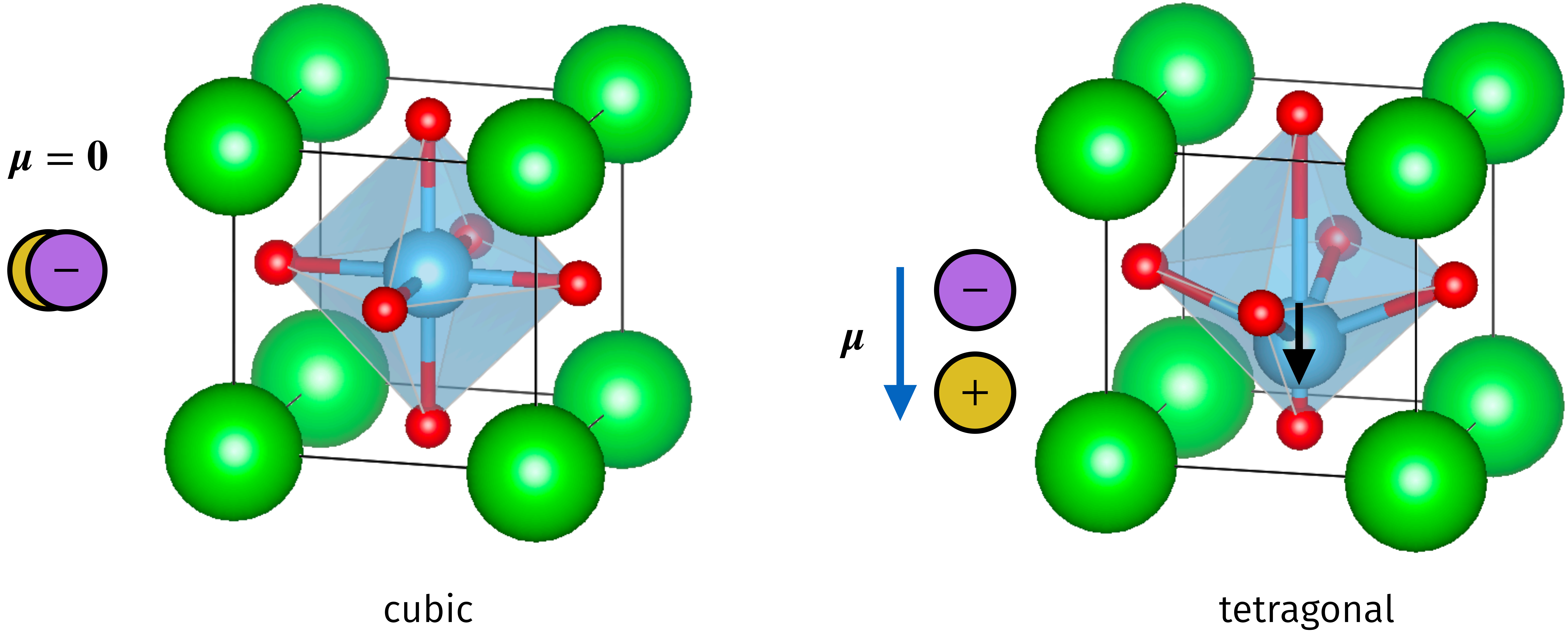


cubic



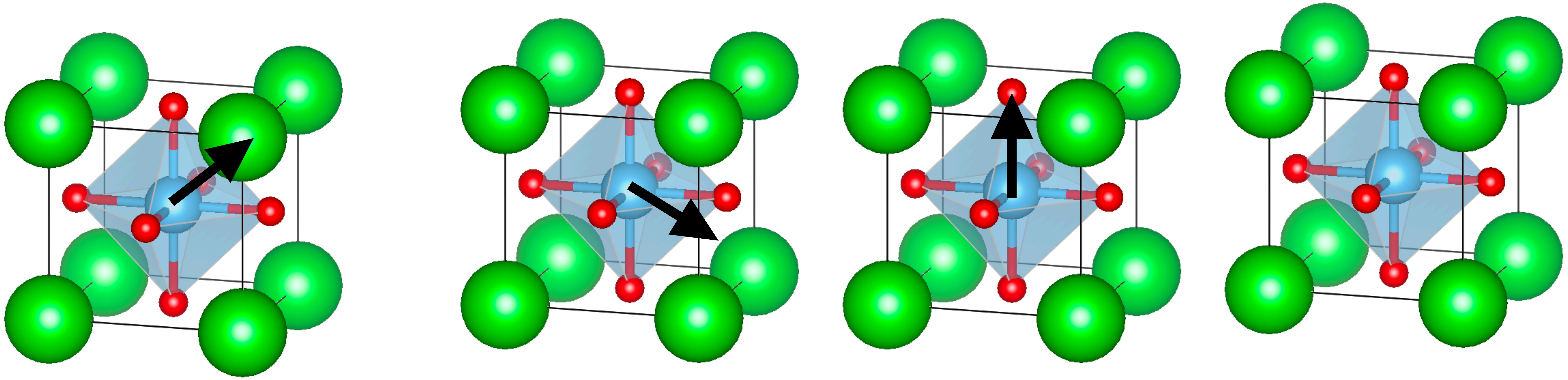
tetragonal

Perovskite structure ABO_3



Phase diagram of $BaTiO_3$

rhombohedral	orthorhombic	tetragonal	cubic
$a = b = c$	$a \neq b \neq c$	$a = b \neq c$	$a = b = c$
$\alpha = \beta = \gamma \neq 90^\circ$	$\alpha = \beta = \gamma = 90^\circ$	$\alpha = \beta = \gamma = 90^\circ$	$\alpha = \beta = \gamma = 90^\circ$



$\langle 111 \rangle$ distortion

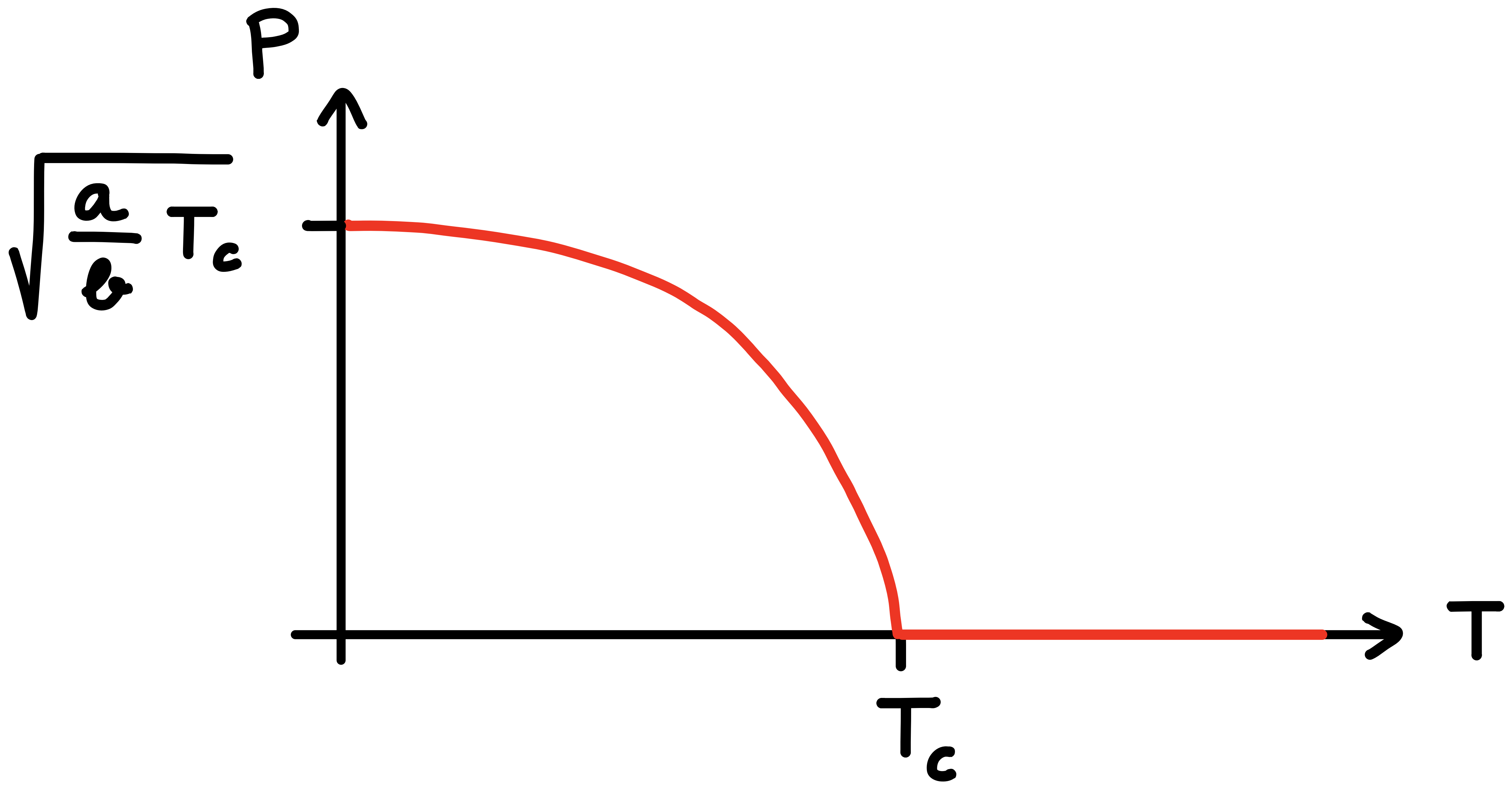
$\langle 110 \rangle$ distortion

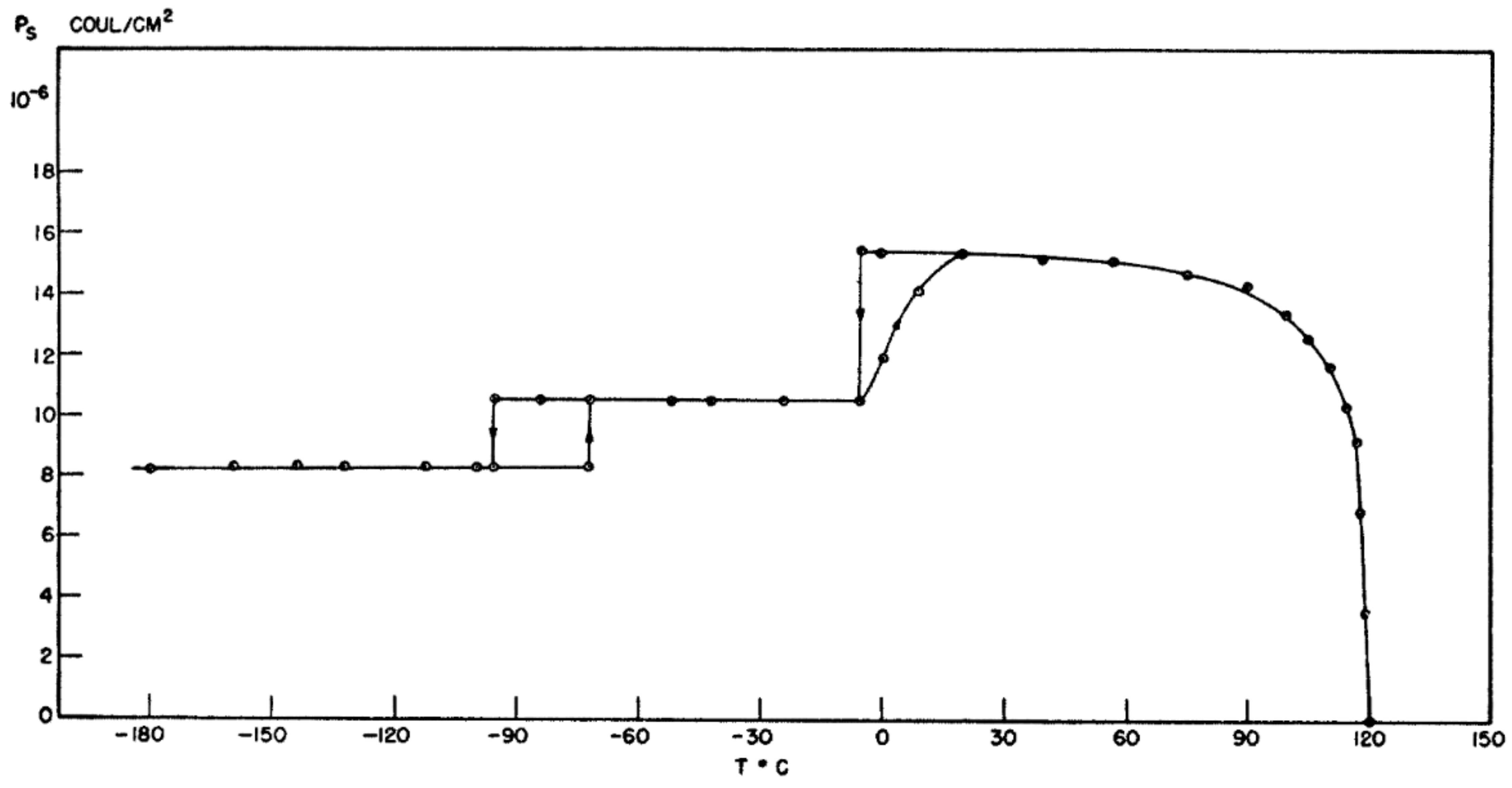
$\langle 100 \rangle$ distortion

T[K]: 0, 183, 278, 393

T[°C]: −273, −90, 5, 120

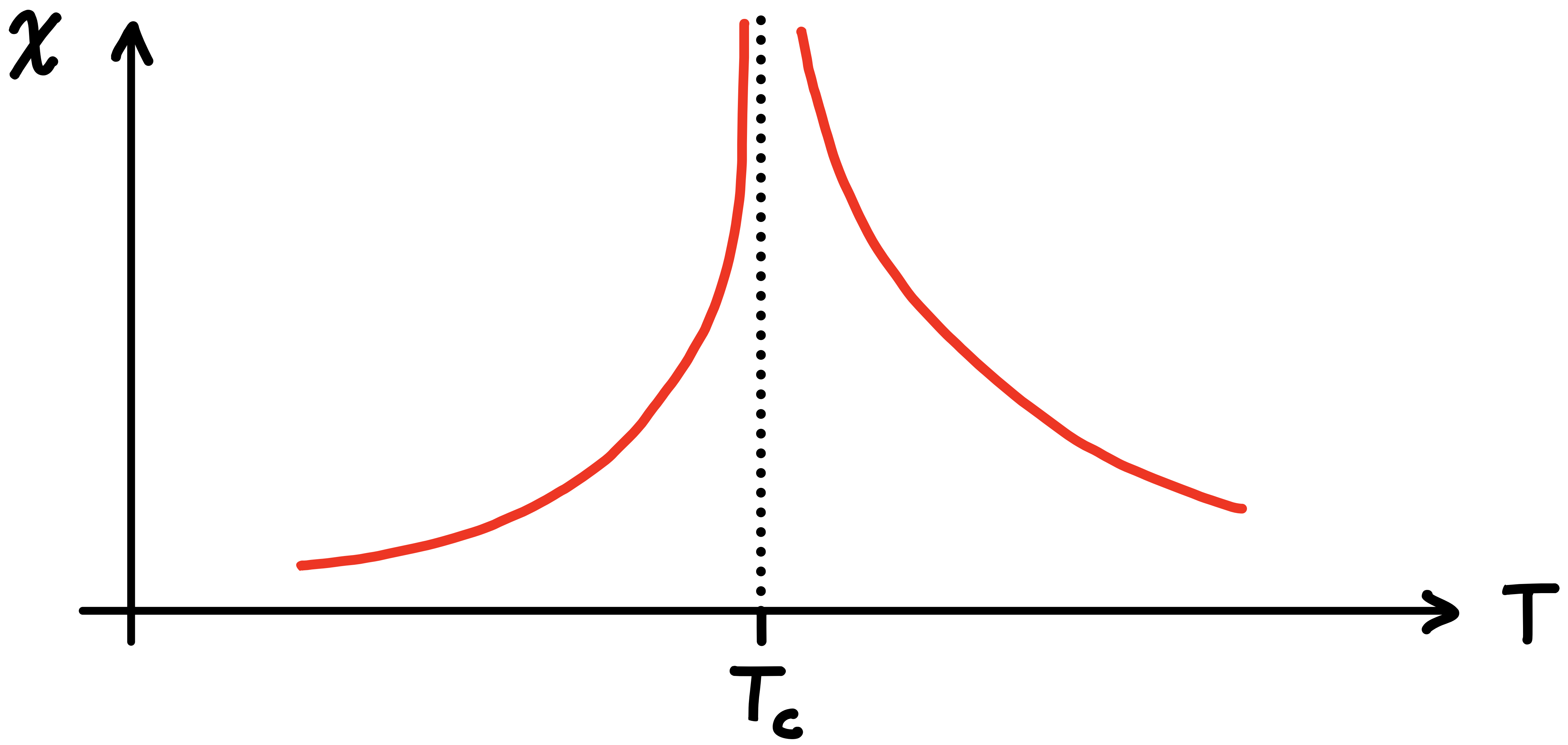
Experimental data for $BaTiO_3$

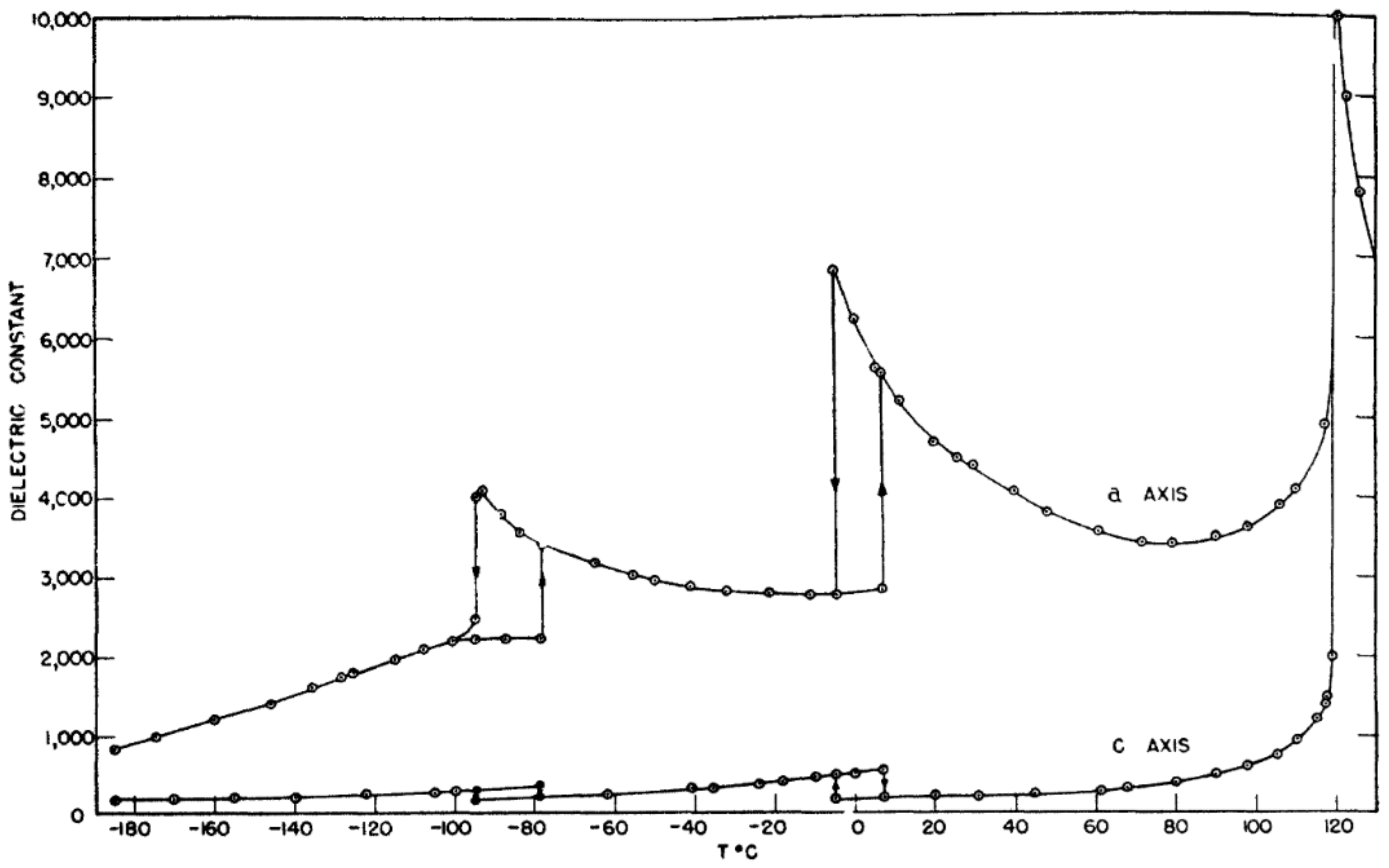




Merz, Physical Review 76, 1221 (1949)

Experimental data for $BaTiO_3$





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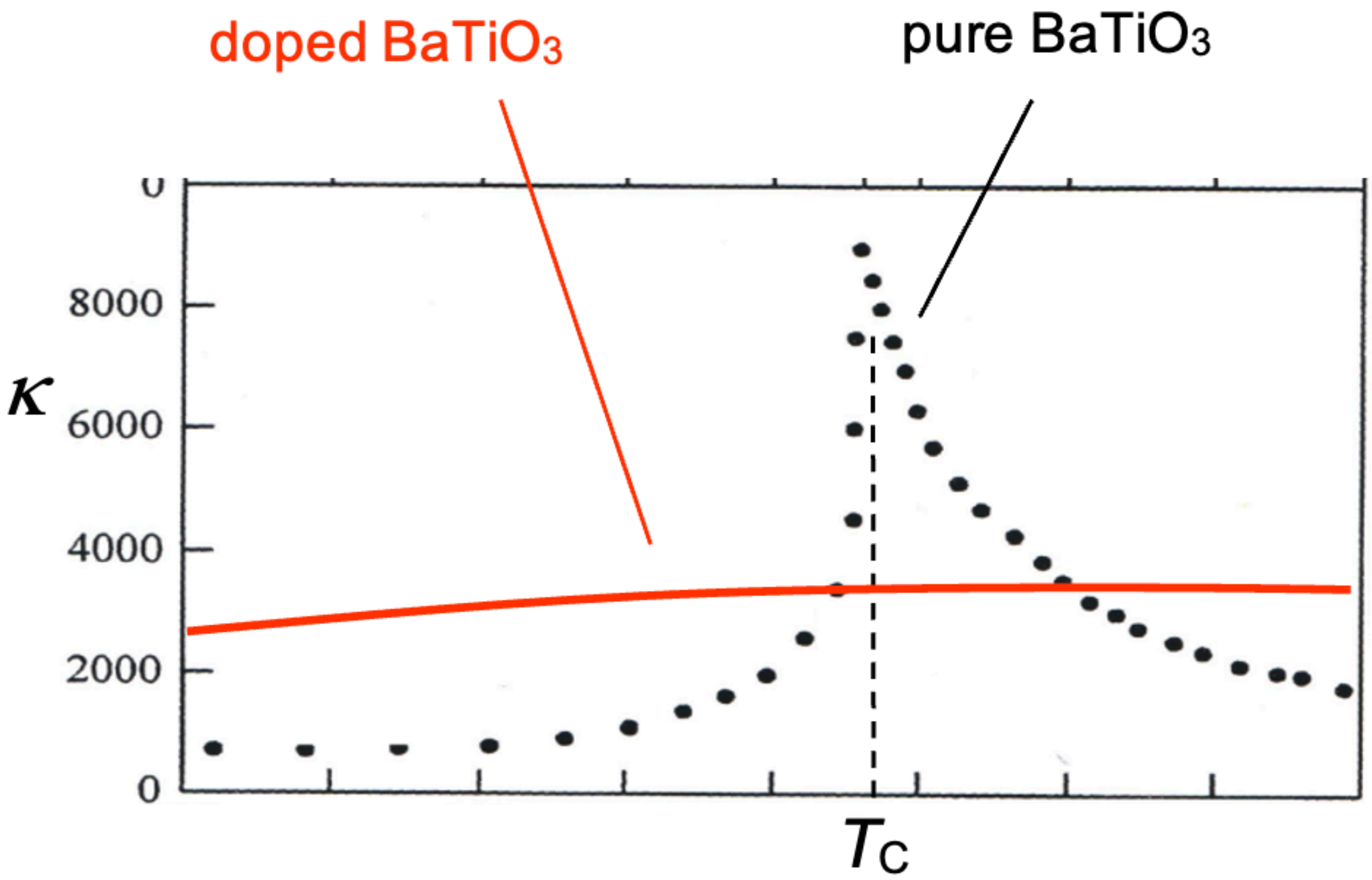
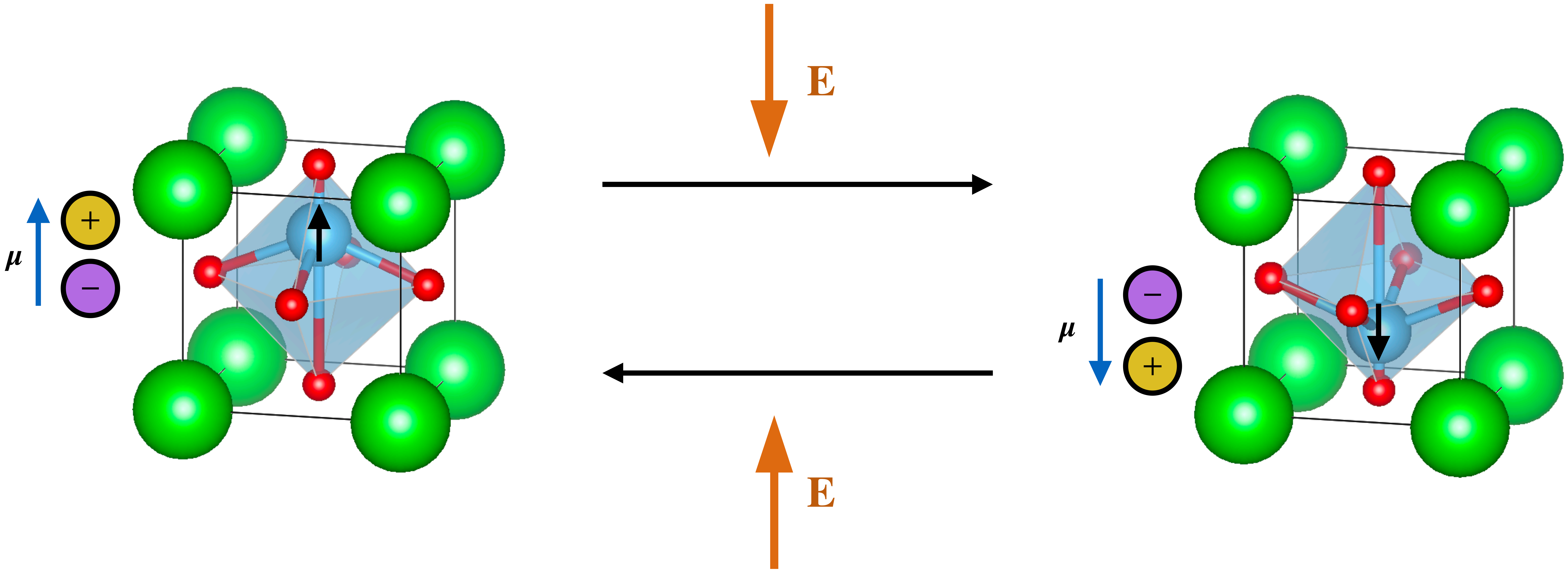
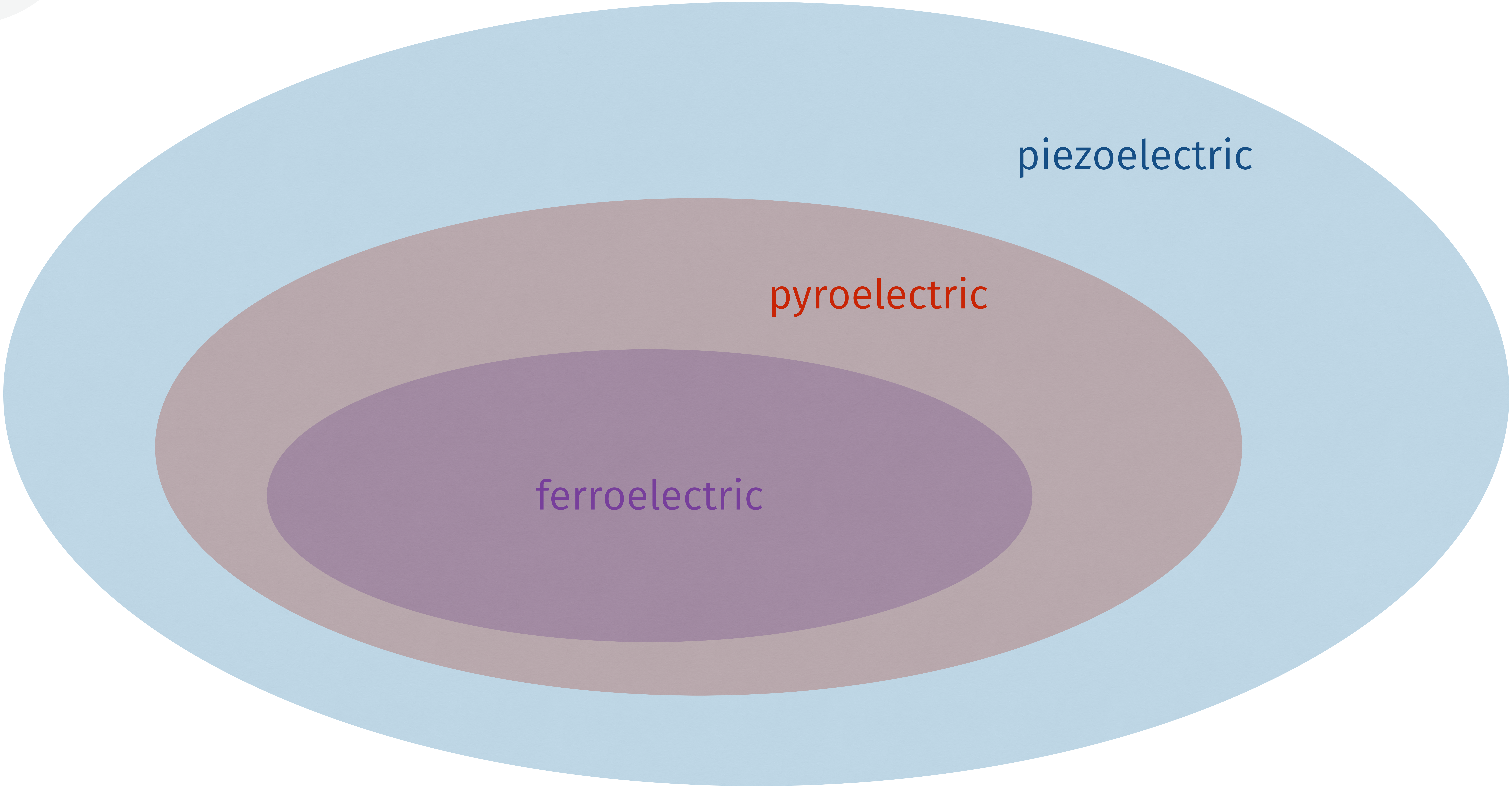
Experimental data for $BaTiO_3$



Ferroelectricity

- Ferroelectricity: spontaneous polarisation that can be reversed by electric field




piezoelectric
pyroelectric
ferroelectric