What is **Negative Capacitance**?

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DRC 2019, June 24, 2019

Semiconductor Research Corporation

Global Research Collaboration

What is Negative Capacitance? (*Is* it real?)

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Is a negative capacitance is a <u>real, physical phenomenon</u> or an <u>unphysical, artificial construct</u> of the phenomenology of the Landau Theory?

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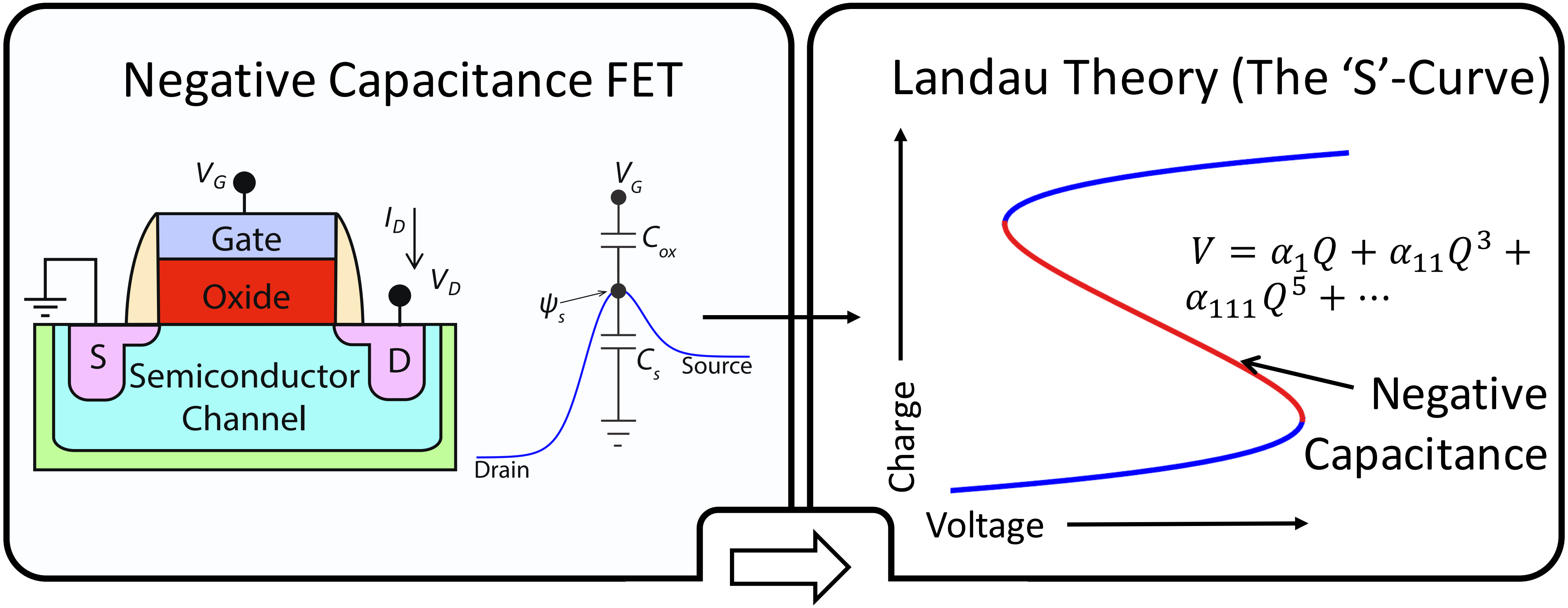
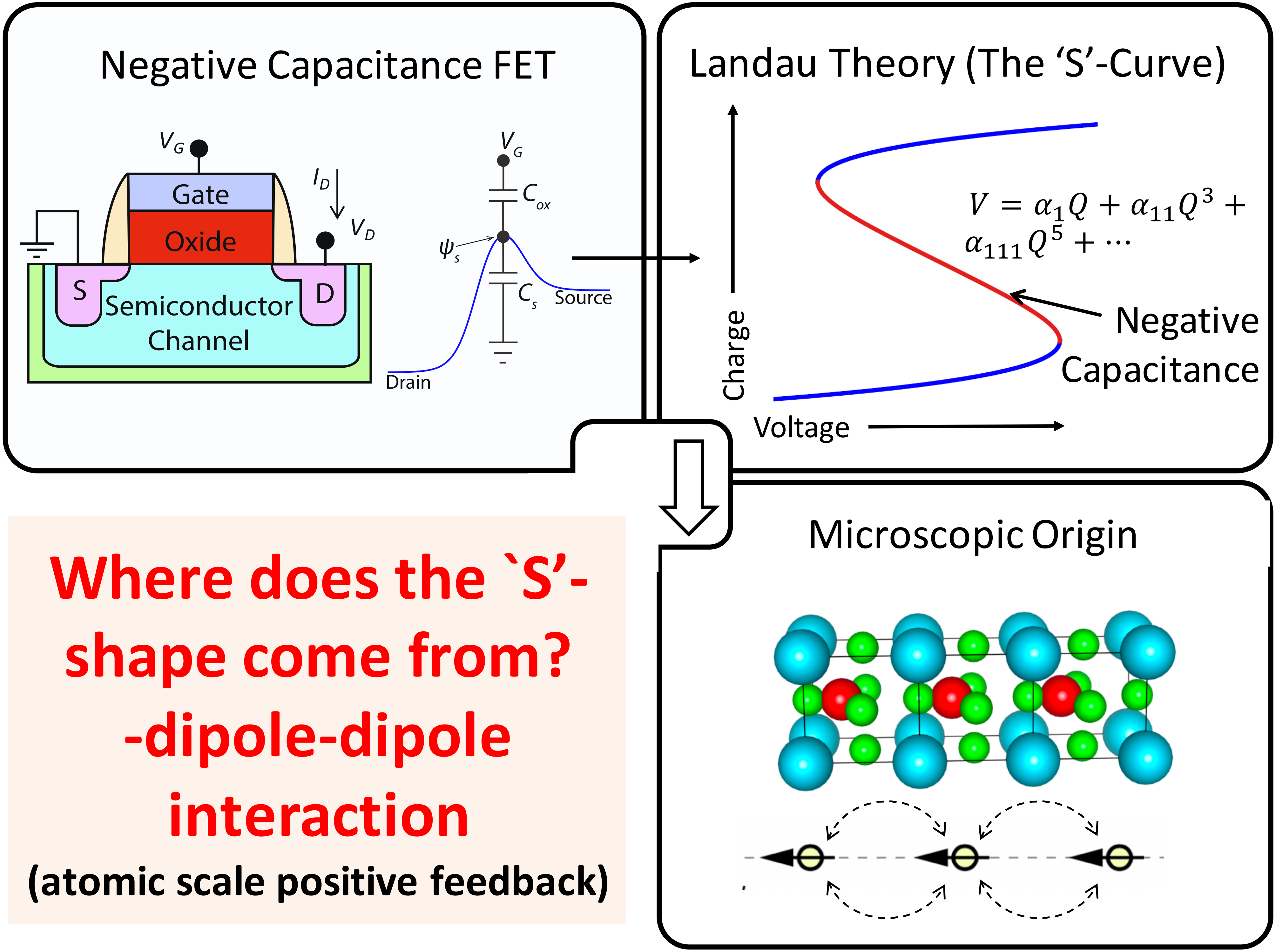


Where does the `S'-shape come from?
-Microscopically

(Landau theory is phenomenological.)


Negative Capacitance FET
V_G
Gate
Oxide
I_D
V_D
S
D
Semiconductor Channel
V_G
C_{ox}
ψ_s
C_s
Source
Drain
Landau Theory (The 'S'-Curve)
$V = \alpha_1 Q + \alpha_{11} Q^3 + \alpha_{111} Q^5 + \cdots$
Negative Capacitance
Charge
Voltage
Microscopic Origin
Where does the `S'-shape come from?
-dipole-dipole interaction
(atomic scale positive feedback)

Is a negative capacitance is a <u>real, physical phenomenon</u> or an <u>unphysical, artificial construct</u> of the phenomenology of the Landau Theory?

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A Ferroelectric **cannot** exist without negative capacitance (i.e., static negative dielectric permittivity).

No Neg-C
No Ferro-E

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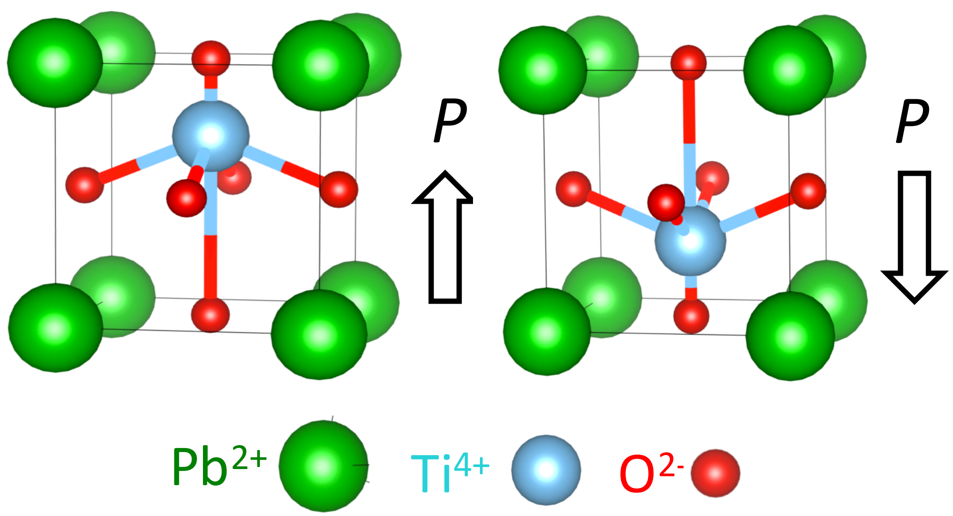
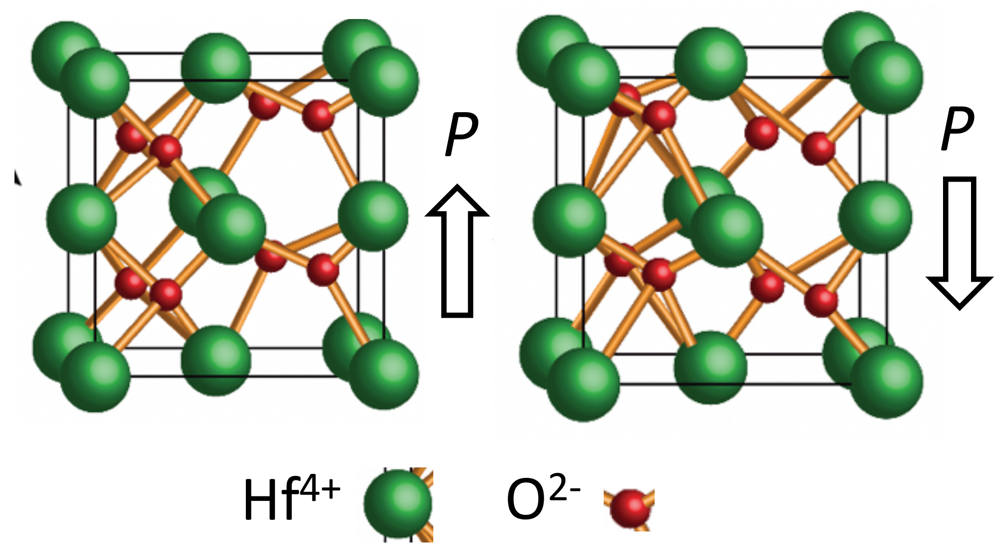
Ferroelectric Oxides

Perovskite Ferroelectric
$PbTiO_3$ ($Pb^{2+}Ti^{4+}O_3^{6-}$)



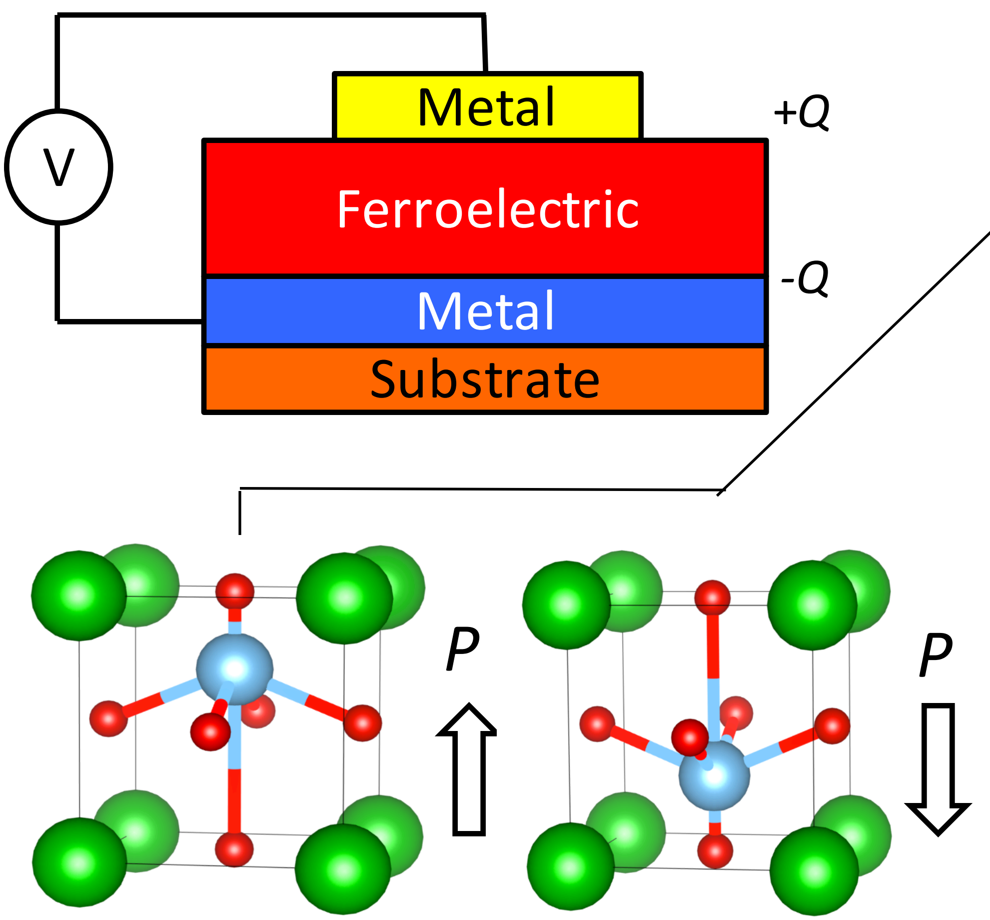
Fluorite-type Ferroelectric
HfO_2 ($Hf^{4+}O_2^{4-}$)



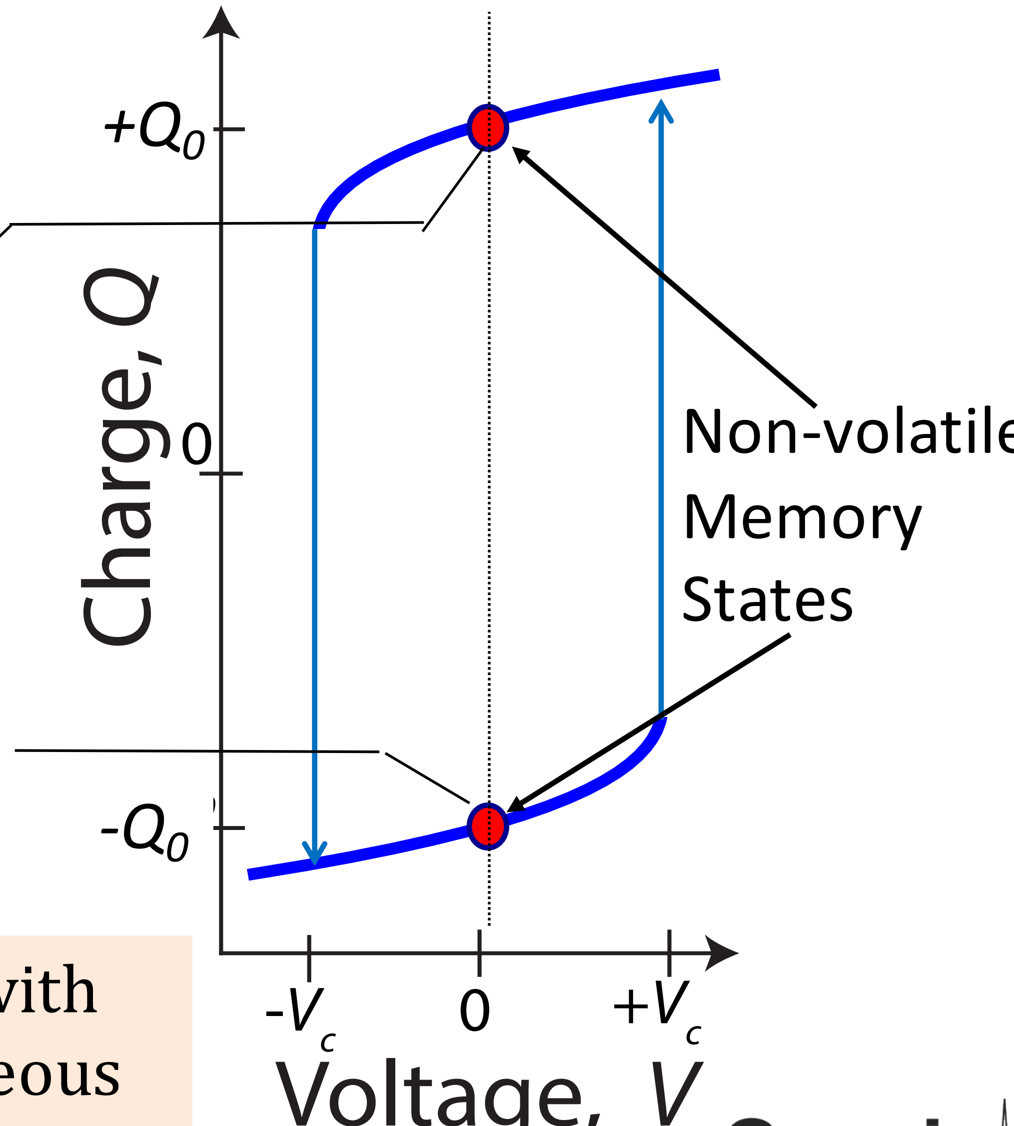
A ferroelectric is an insulator with a spontaneous polarization, which can be switched by an above coercive voltage .

Ferroelectric Oxides

Ferroelectric Capacitor



Charge-Voltage Characteristics



A ferroelectric is an insulator with electrically switchable spontaneous polarization.

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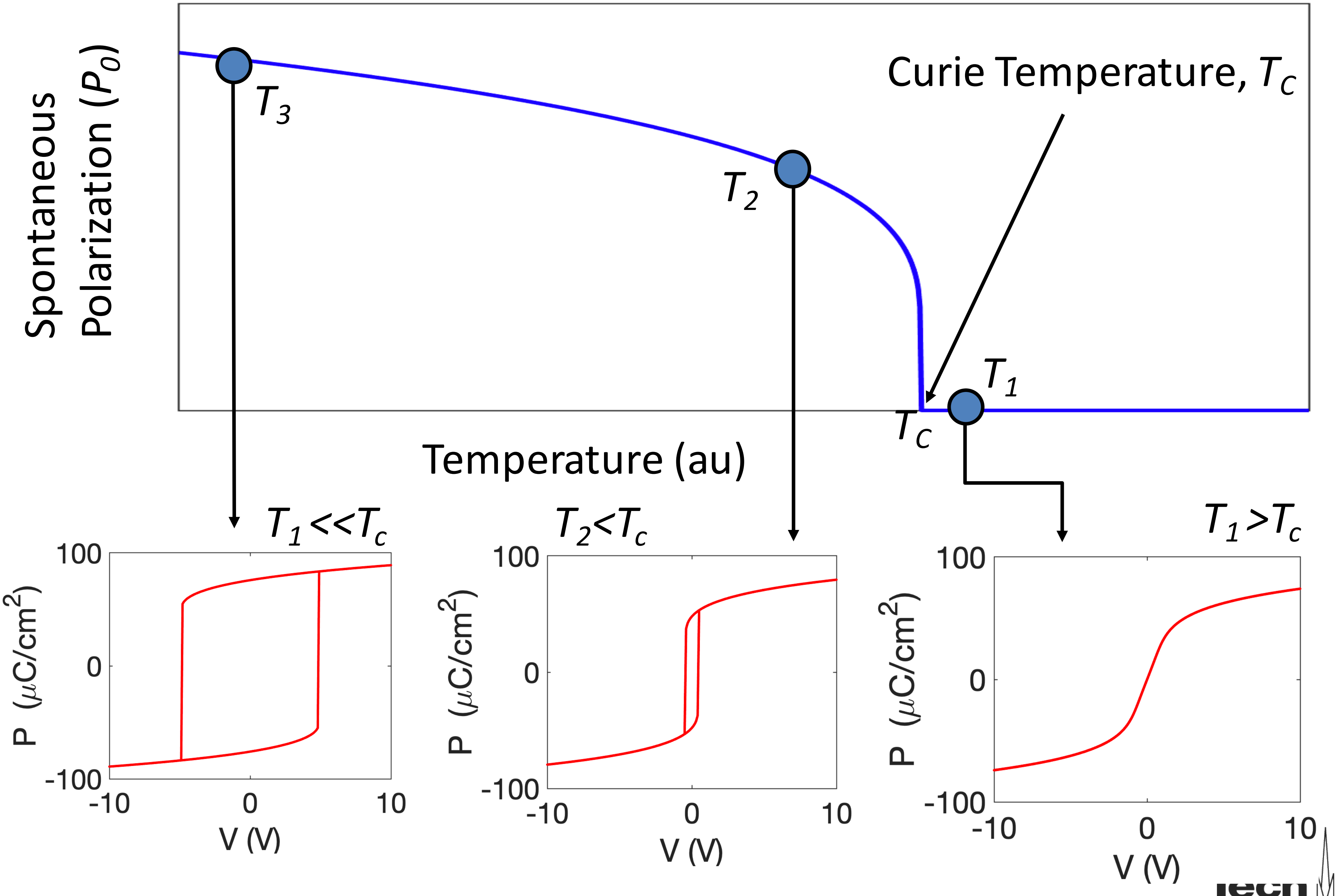
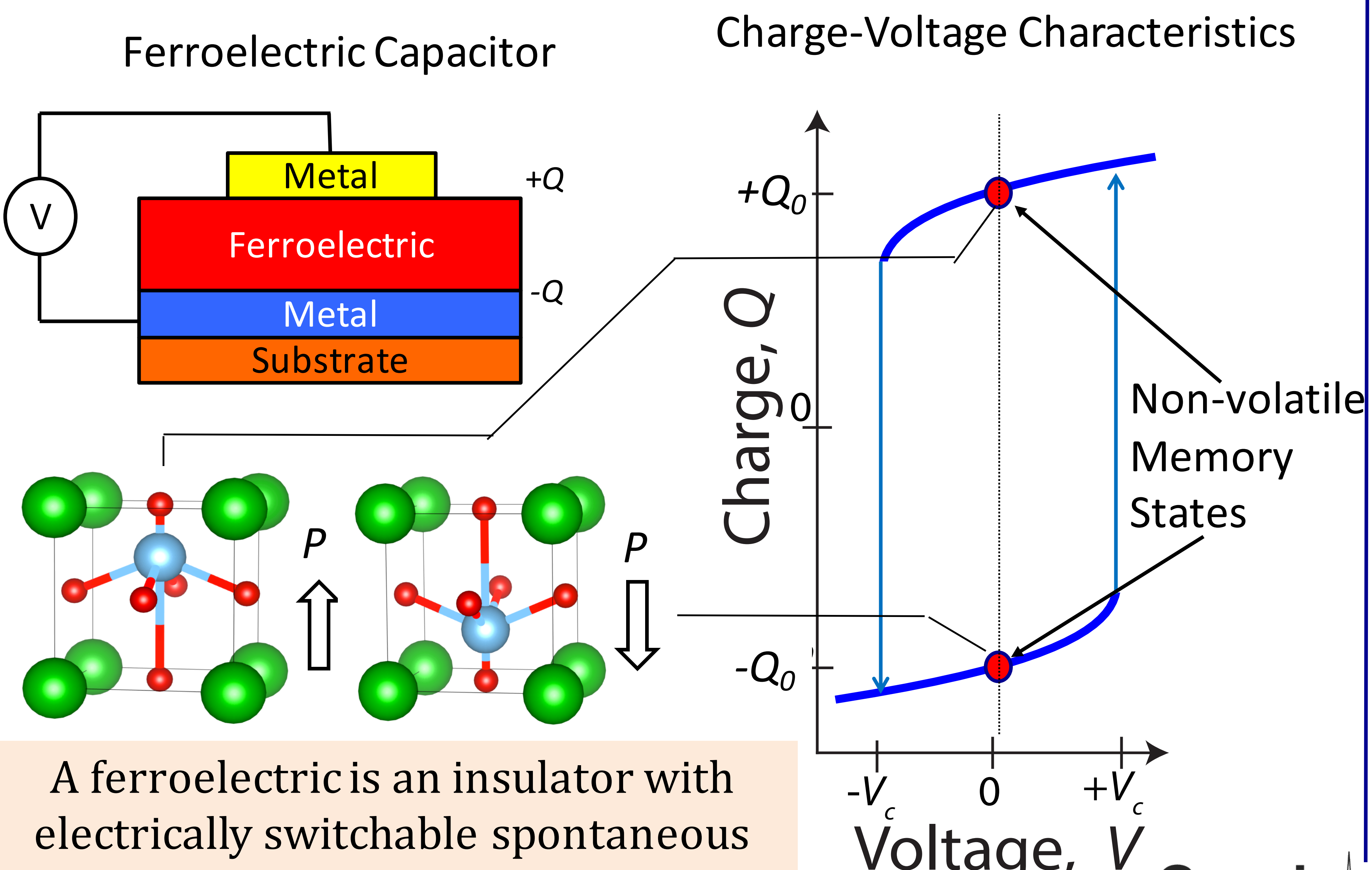
Ferroelectric Oxides: Temperature dependence



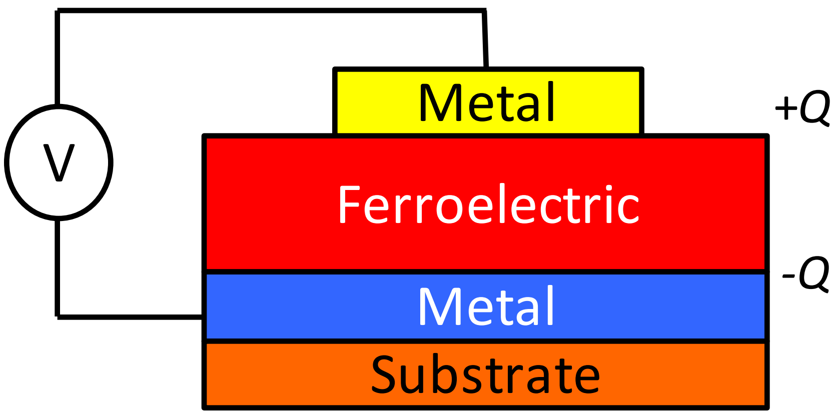
Ferroelectric Oxides



A ferroelectric is an insulator with electrically switchable spontaneous polarization.

Ferroelectric Oxides: Landau Theory

Ferroelectric Capacitor



$$V = \alpha_1 Q + \alpha_{11} Q^3 + \alpha_{111} Q^5 + \cdots$$

$\alpha_1 = a_0(T - T_c) < 0$ below T_c

T = temperature

T_c =Curie temperature

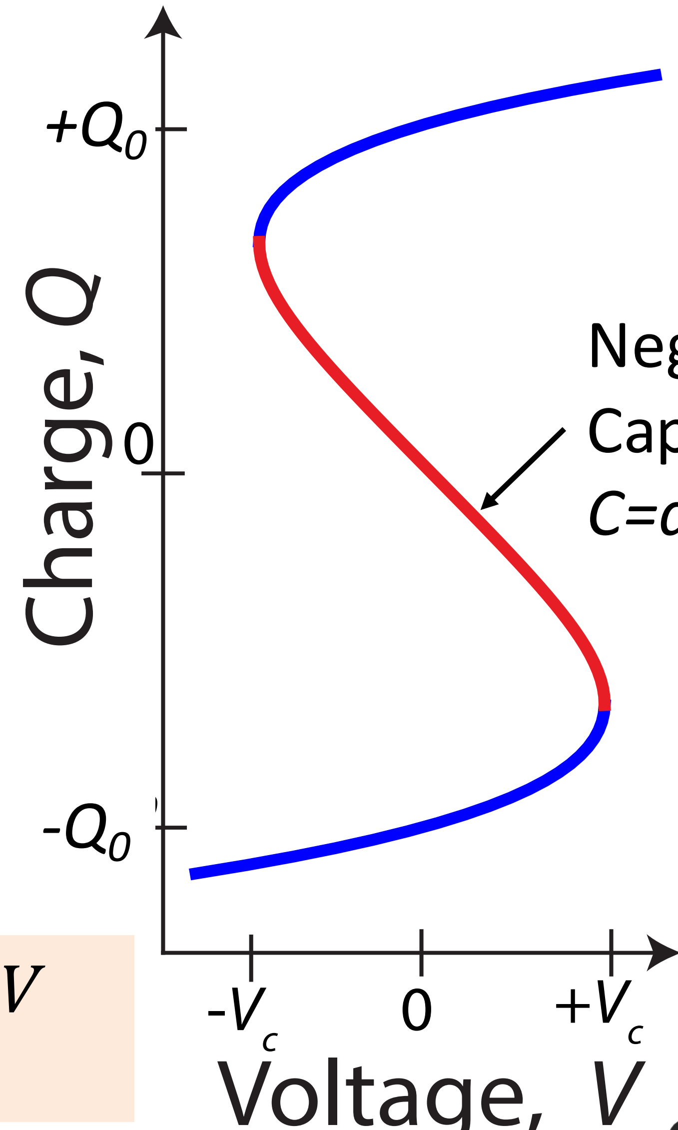
a_0 =positive constant

α_{11}=positive (2nd order) or negative (1st order)

α_{111} =positive

Landau theory: In certain Q and V range, $C=dQ/dV$ is begative

Charge-Voltage Characteristics



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History of Landau theory of ferroelectrics

1937: Lev Landau first proposes the framework for phase transition

L. D. Landau, Phys. Z. Sowjun, vol. 11, pp. 545, 1937.; "On the theory of phase transitions. II," Zh. Eksp. Teor. Fiz. Vol. 7, pp. 627, 1937

Late 1940s: Ginzburg and Devonshire applies Landau theory to ferroelectrics after discovery of ferroelectricity in $BaTiO_3$

V. L. Ginzburg, Zh. Eksp. Teor. Fiz., vol. 15, pp. 739, 1945; V. L. Ginsburg, J. Phys. USSR, vol. 10, pp.107, 1946.

A. F. Devonshire: Philos. Mag., vol. 40, pp. 1040, 1949.

Landau framework is <u>phenomenological</u> mean-field theory based on symmetry to analyze phase transitions.

-Connects microscopic models to macroscopic behavior

<u>But does not talk about underlying microscopic origin!</u>

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History of Landau theory of ferroelectrics

'S'-shape in polarization-electric field curve appeared in early papers in 1950s on the Landau Theory of Ferroelectrics!

But negative capacitance region in ferroelectric was <u>not explicitly discussed</u> except for asserting that this region is "thermodynamically unstable."

Merz
Physical Review, 1953.

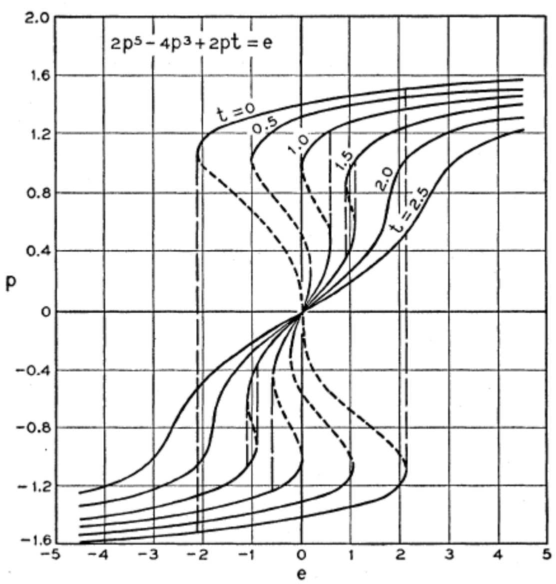
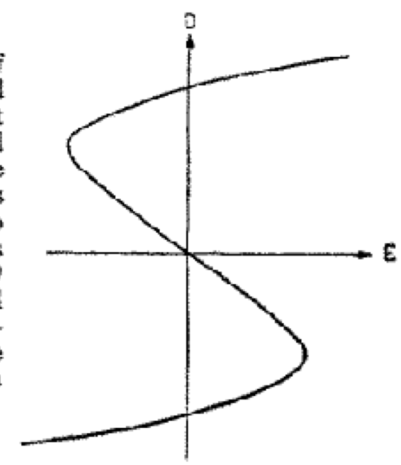


FIG. 3. Plot of function $2p^5-4p^3+2pt=e$.

R. Landauer
J. Appl. Phys, 1957.

FIG. 4. General form of relationship between D and E for barium titanate at room temperature. D and E are taken to be along the c axis and the crystal is assumed to be clamped to the dimensions that it has in the absence of a field. D and $4\pi P$ are almost equal and this curve has essentially the same shape as the P vs E relationship for a "clamped" crystal.



Janovec
Czech. fiz. zurnal, 1959.

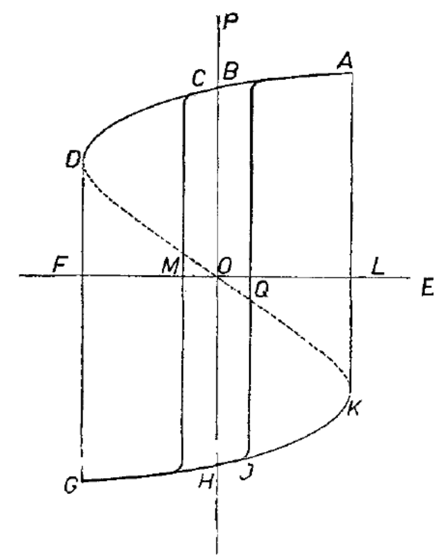
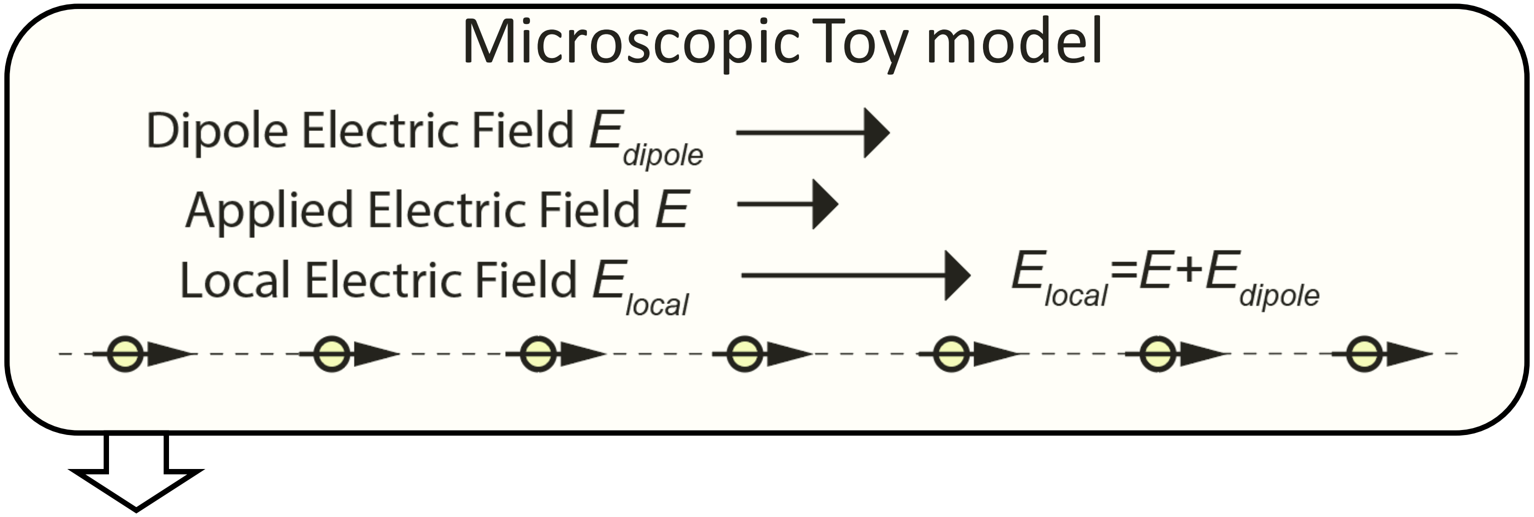
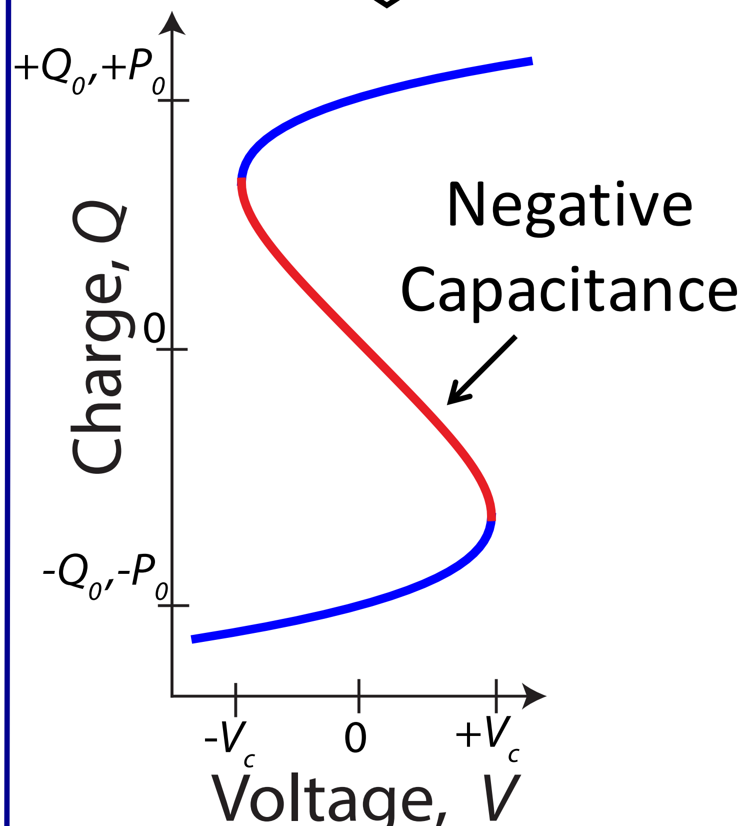


Fig. 1. Hysteresis dependence of polarisation P on intensity of electric field E.

Toy model of Negative Capacitance ('S'-curve)

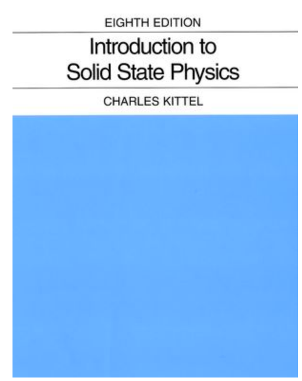


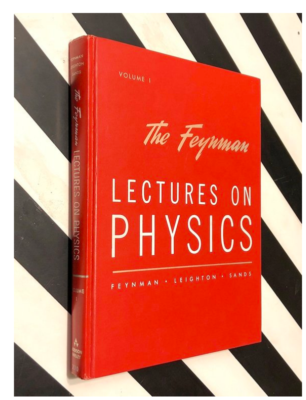


-Simple, physical explanation of underlying microscopic mechanisms of ferroelectric negative

-Electrostatic dipole-dipole interactions

-Atomic scale positive feedback mechanism





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Toy model of Negative Capacitance (‘S’-curve)

Dipole Electric Field E_{dipole}

Applied Electric Field E

Local Electric Field E_{local}

$E_{local}=E+E_{dipole}$

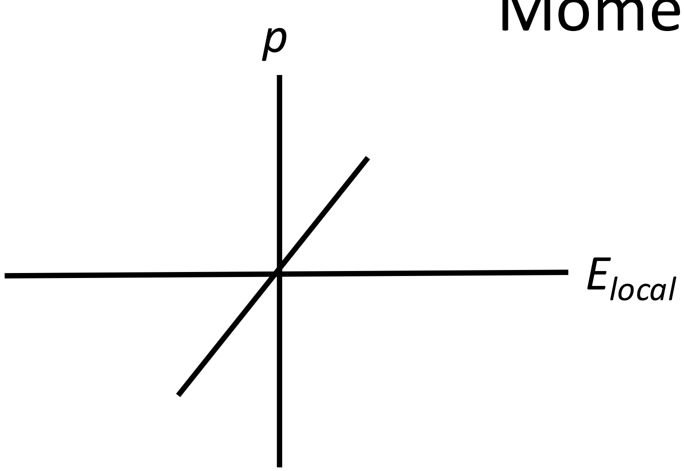
Polarizability

a

Dipole Moment

$$p = \alpha\epsilon_0 E_{local}$$

Vacuum Permittivity

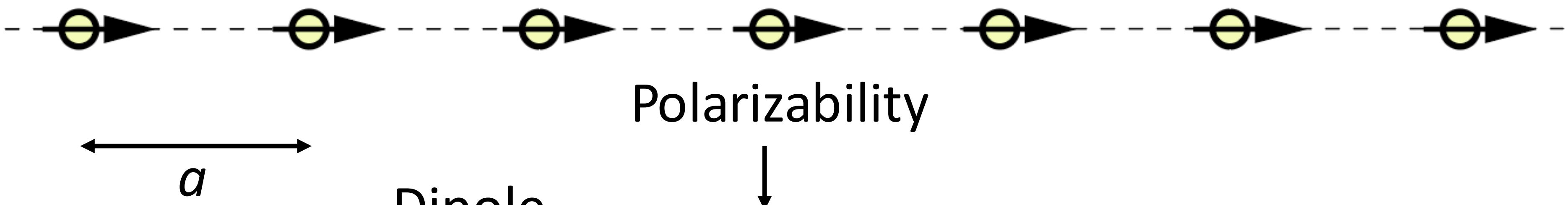


Toy model of Negative Capacitance (‘S’-curve)

Dipole Electric Field E_{dipole} →

Applied Electric Field E →

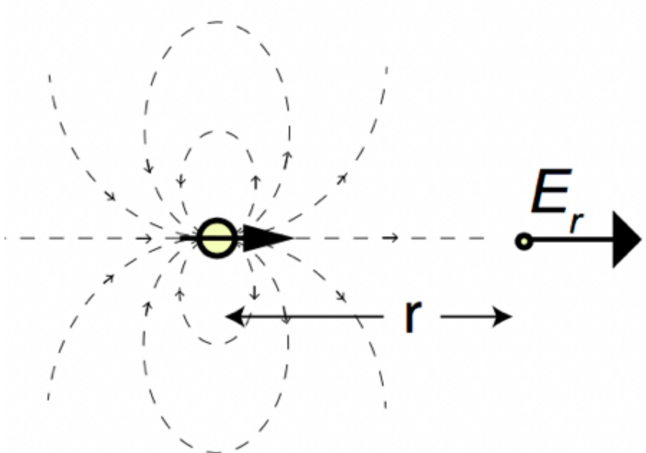
Local Electric Field E_{local} → $E_{local}=E+E_{dipole}$



Polarizability

Dipole Moment $p = \alpha\epsilon_0 E_{local}$

Vacuum Permittivity



$$E_r = \frac{1}{4\pi\epsilon_0}\frac{2p}{r^3}$$

Toy model of Negative Capacitance ('S'-curve)

Dipole Electric Field E_{dipole}

Applied Electric Field E

Local Electric Field E_{local}

$E_{local}=E+E_{dipole}$

a

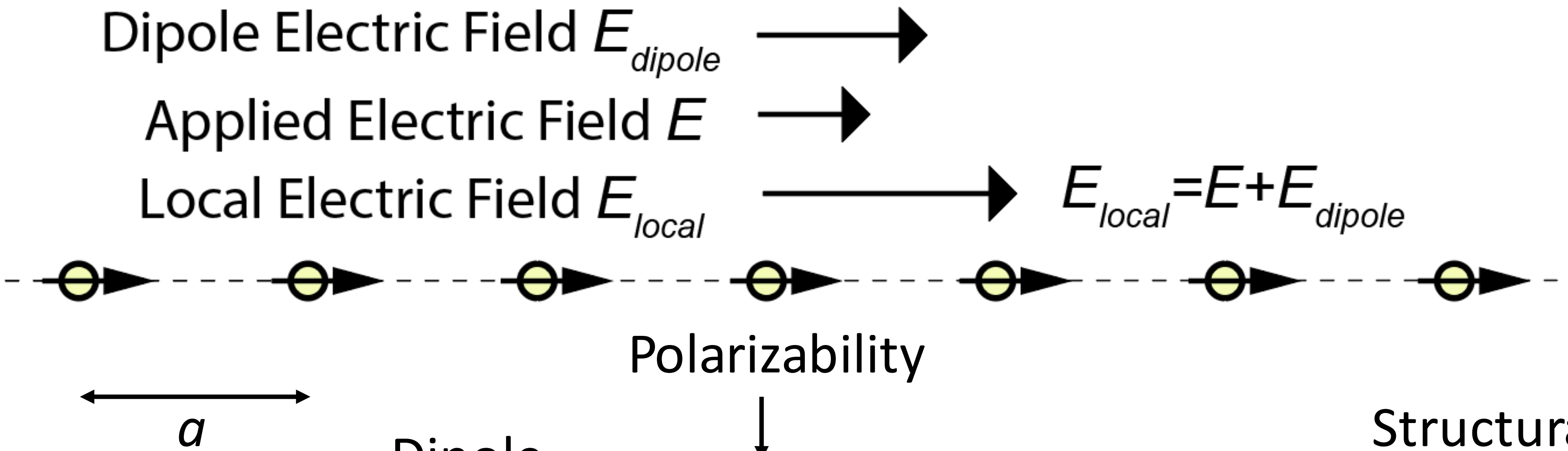
Polarizability

Dipole Moment $p = \alpha \epsilon_0 E_{local}$

Structural Factor

$$E_{dipole} = 2\times \frac{1}{4\pi\epsilon_0}\frac{2p}{a^3}\left(1+\frac{1}{2^3}+\frac{1}{3^3}+\cdots\right) = \frac{p}{\epsilon_0}\frac{0.383}{a^3} = \zeta p$$

Toy model of Negative Capacitance ('S'-curve)



Polarizability

Dipole Moment $p = \alpha \epsilon_0 E_{local}$

Structural Factor

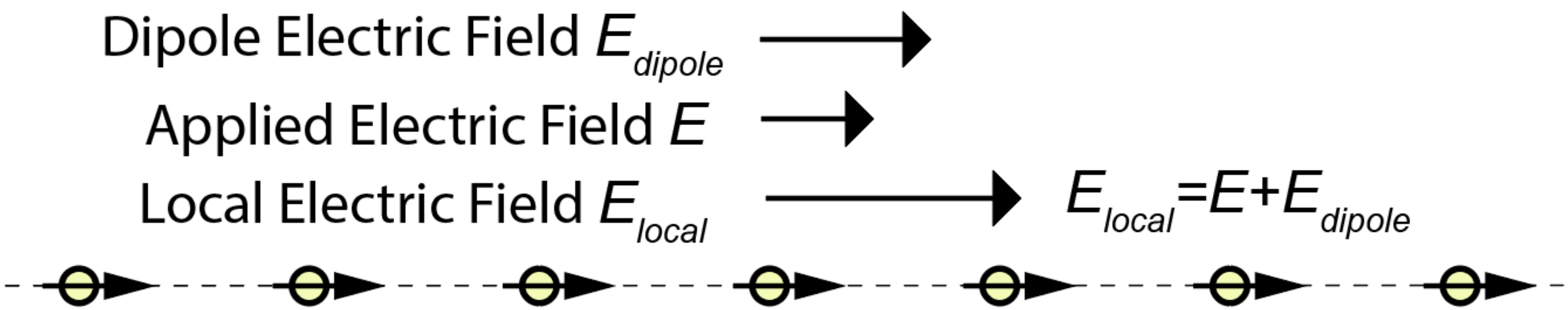
$$E_{dipole} = 2 \times \frac{1}{4\pi\epsilon_0} \frac{2p}{a^3} \left(1 + \frac{1}{2^3} + \frac{1}{3^3} + \cdots \right) = \frac{p}{\epsilon_0} \frac{0.383}{a^3} = \zeta p$$

$$E_{local} = E_{dipole} + E$$

Atomic scale feedback

1. Dipole moment depends on local electric field.
2. Local electric field depends on dipole moment.

Toy model of Negative Capacitance (‘S’-curve)



Atomic scale feedback

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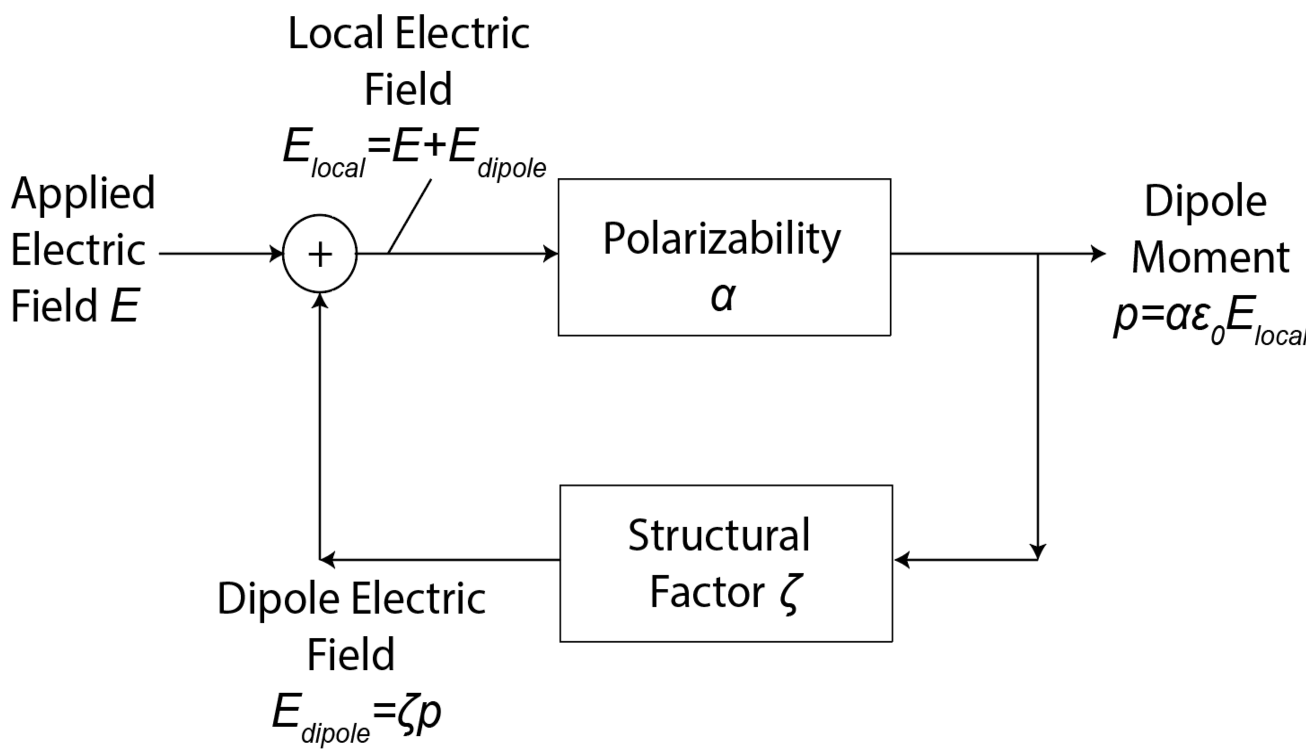


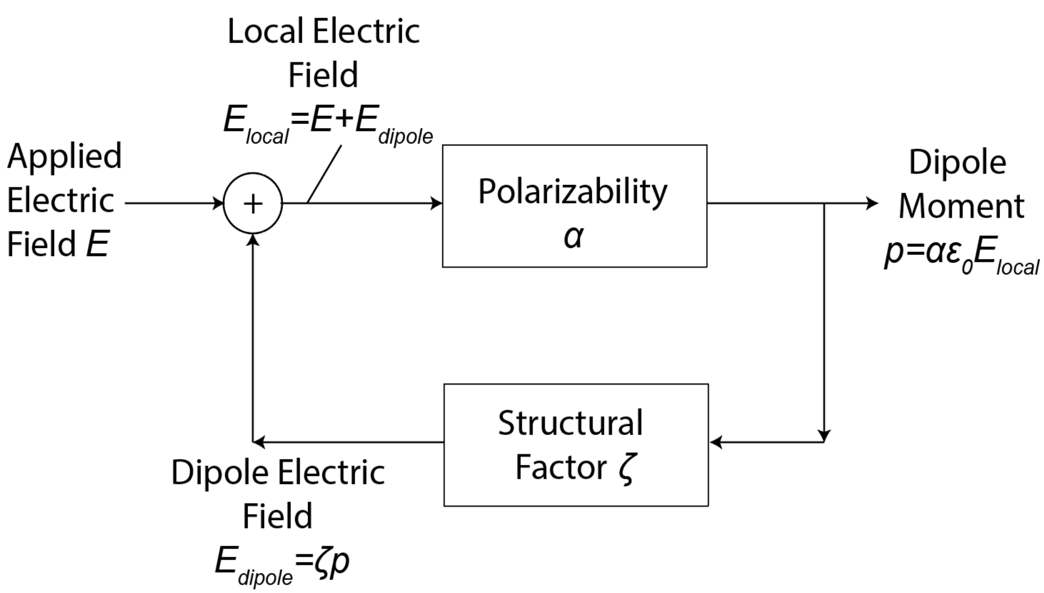
Toy model of Negative Capacitance ('S'-curve)

Dipole Electric Field E_{dipole}

Applied Electric Field E

Local Electric Field E_{local}

$E_{local}=E+E_{dipole}$



Dipole moment

$$p = \alpha\epsilon_0 E_{local}$$

Dipole field

$$E_{dipole} = \zeta p$$

Local field

$$E_{local} = E_{dipole} + E$$

$$p = \alpha\epsilon_0(\zeta p + E)$$

Dipole moment: $p = \dfrac{\alpha\epsilon_0}{1-\alpha\epsilon_0\zeta}\mathrm{E}$

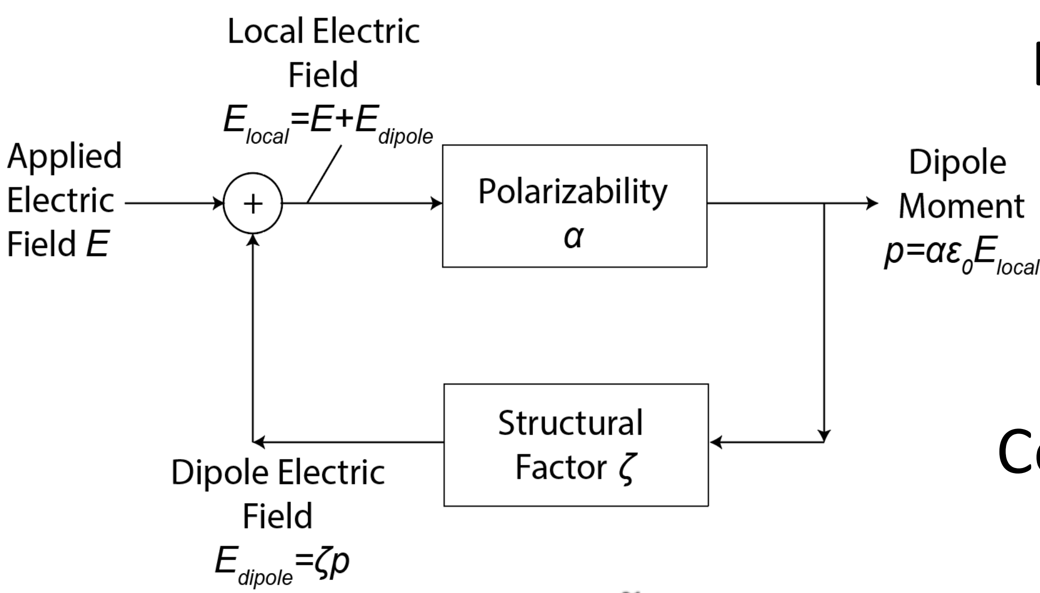
Toy model of Negative Capacitance (‘S’-curve)

Dipole Electric Field E_{dipole}

Applied Electric Field E

Local Electric Field E_{local}

$E_{local}=E+E_{dipole}$



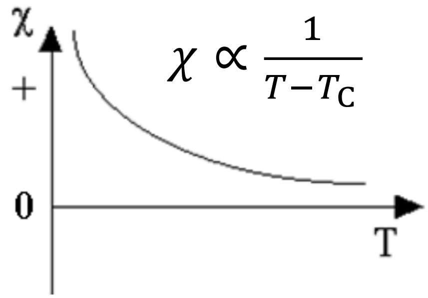
Dipole moment: $p = \frac{\alpha\epsilon_0}{1-\alpha\epsilon_0\zeta}\mathrm{E}$

$$\alpha = \frac{1}{\gamma\epsilon_0 T}$$

Constant Temp.

$$\zeta = \gamma T_C$$

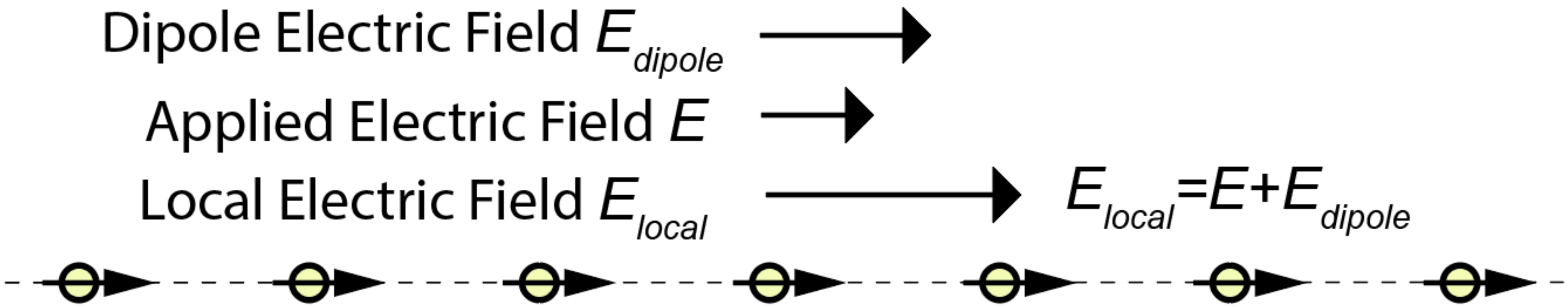
Curie Temp.



$$\frac{dp}{dE} = \frac{\alpha\,\epsilon_0}{1-\alpha\,\epsilon_0\zeta} \propto \frac{1}{T-T_C}$$

Curie-Weiss Law

Toy model of Negative Capacitance ('S'-curve)



Dipole moment: $p = \frac{\alpha\epsilon_0}{1-\alpha\epsilon_0\zeta}\mathrm{E}$

$$\frac{dp}{dE} = \frac{\alpha\,\epsilon_0}{1-\alpha\epsilon_0\zeta}$$

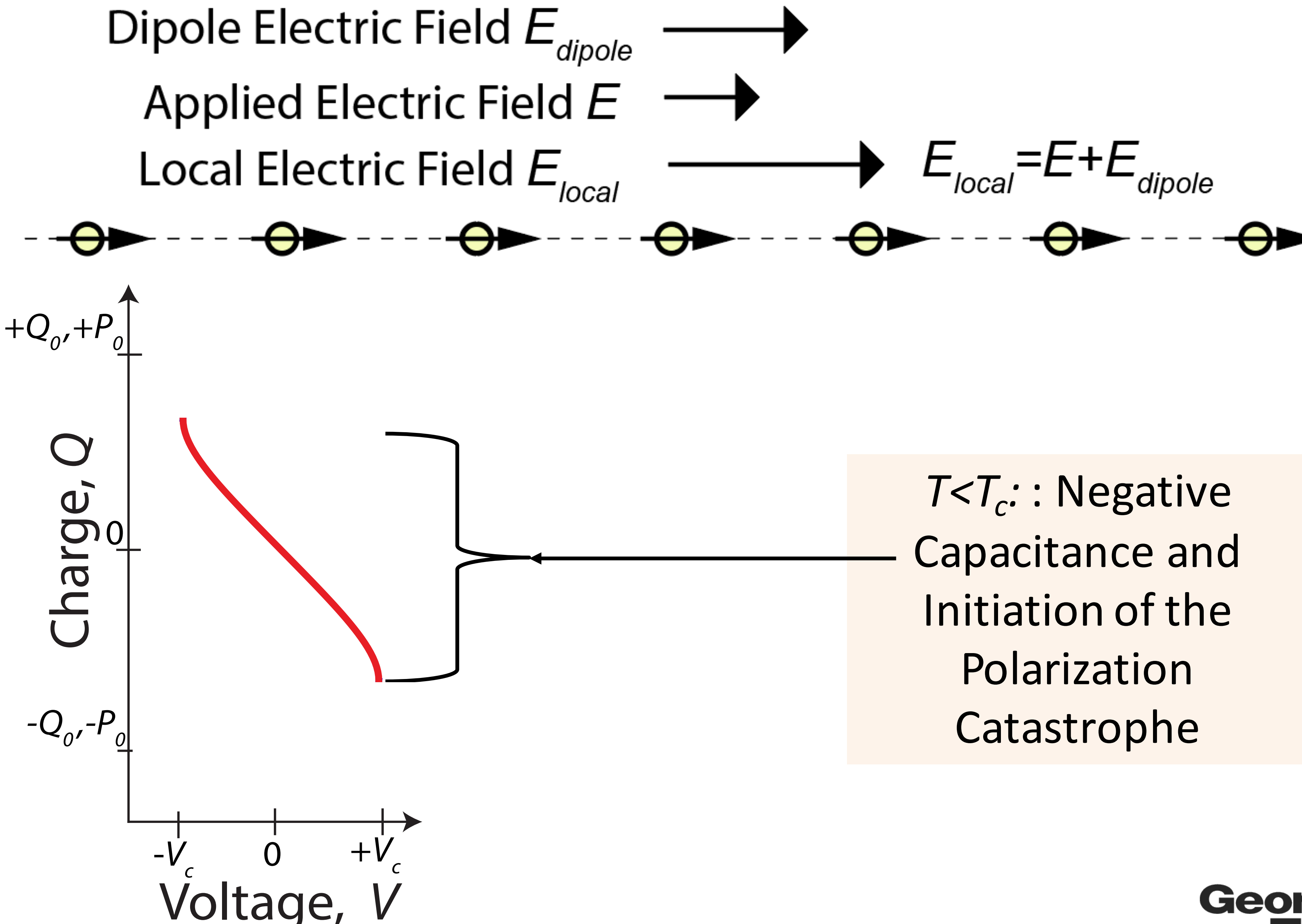
If $\alpha\epsilon_0\zeta > 1$ (if the material is highly polarizable),

$$\frac{dp}{dE} < 0$$

<u>Polarization Catastrophe</u>

The negative dielectric negative capacitance that sets off the polarization catastrophe and leads to the emergence of the spontaneous polarization in ferroelectric material.

Toy model of Negative Capacitance (‘S’-curve)

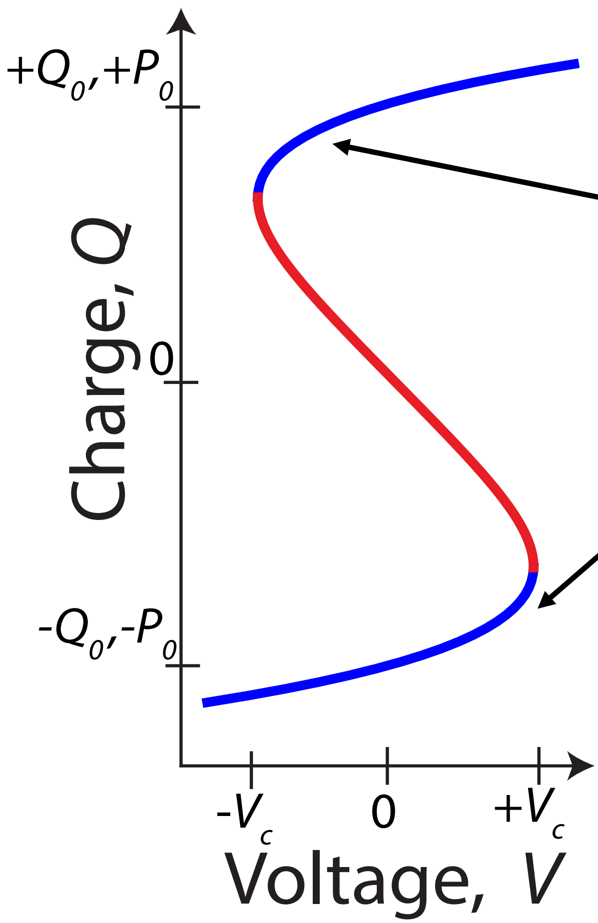


Toy model of Negative Capacitance (‘S’-curve)

Dipole Electric Field E_{dipole} $\longrightarrow$

Applied Electric Field E $\rightarrow$

Local Electric Field E_{local} $\longrightarrow$ $E_{local}=E+E_{dipole}$



How to get the turn-back feature?

Toy model of Negative Capacitance ('S'-curve)

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Applied Electric Field E

Local Electric Field E_{local}

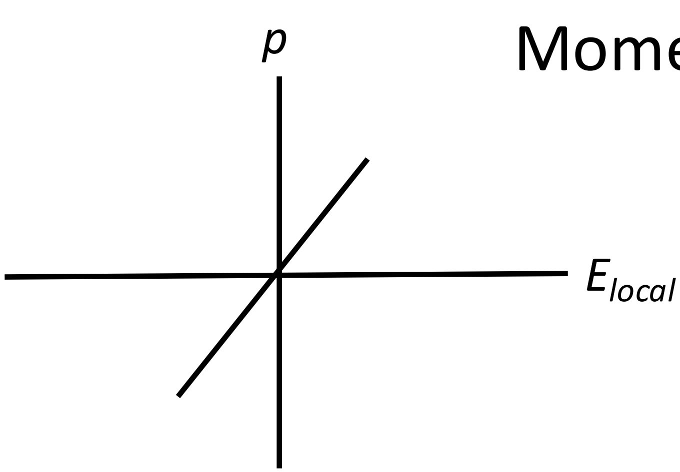
$E_{local}=E+E_{dipole}$

Polarizability

Dipole Moment

$$p = \alpha\epsilon_0 E_{local}$$

Vacuum Permittivity



Toy model of Negative Capacitance (‘S’-curve)

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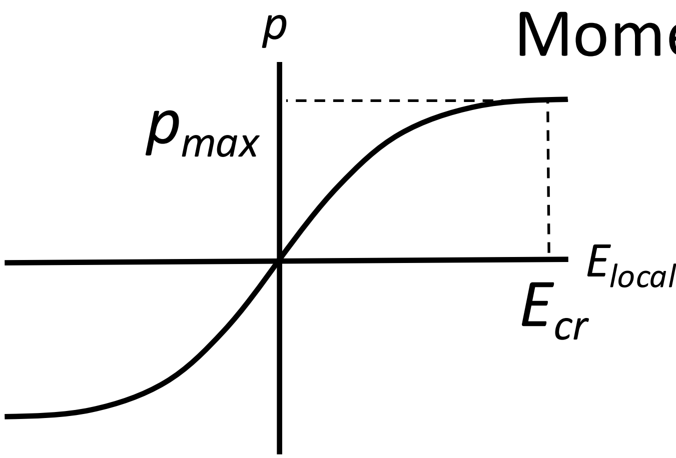
Polarizability

Dipole Moment

$$p = \alpha\epsilon_0 E_{local}$$



Because dipoles are not infinitely polarizable.

Dipole moment: $p = p_{max} \tanh \frac{E_{local}}{E_{cr}}$

Maximum moment: $p_{max} = \alpha\epsilon_0 E_{cr}$

Critical field: E_{cr}

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Toy model of Negative Capacitance ('S'-curve)

Dipole Electric Field E_{dipole}

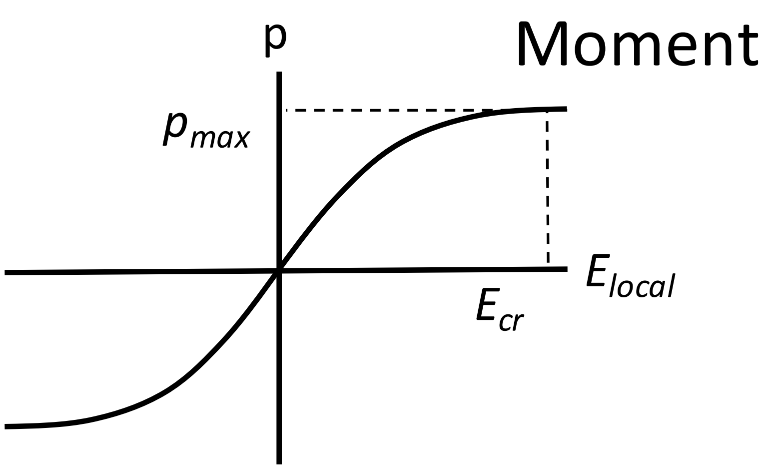
Applied Electric Field E

Local Electric Field E_{local}

$E_{local} = E + E_{dipole}$

Dipole moment: $p = p_{max} \tanh \frac{E_{local}}{E_{cr}}$

Maximum moment: $p_{max} = \alpha \epsilon_0 E_{cr}$



Polarizability

$$\alpha = \frac{1}{\underbrace{\gamma \epsilon_0}_{\text{Constant}} \underbrace{T}_{\text{Temperature}}}$$

Structural Factor

$$\zeta = \gamma \underbrace{T_C}_{\text{Curie Temperature}}$$

Toy model of Negative Capacitance ('S'-curve)

Dipole Electric Field E_{dipole}

Applied Electric Field E

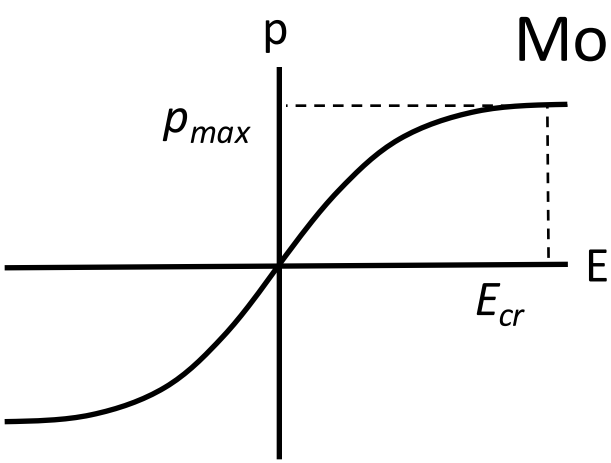
Local Electric Field E_{local}

$E_{local} = E + E_{dipole}$

Dipole moment: $p = p_{max} \tanh \frac{E_{local}}{E_{cr}}$

Maximum moment: $p_{max} = \alpha \epsilon_0 E_{cr}$

Dipole Moment



$$\alpha = \frac{1}{\gamma \epsilon_0 T} \qquad \zeta = \gamma T_C$$

Dipole field

$$E_{dipole} = \zeta p$$

$$E_{local} = E_{dipole} + E$$

$$\frac{E}{E_{cr}} = -\frac{T}{T_c}\frac{p}{p_{max}} + \frac{1}{2}\log\frac{1 + {}^{p}/_{p_{max}}}{1 - {}^{p}/_{p_{max}}}$$

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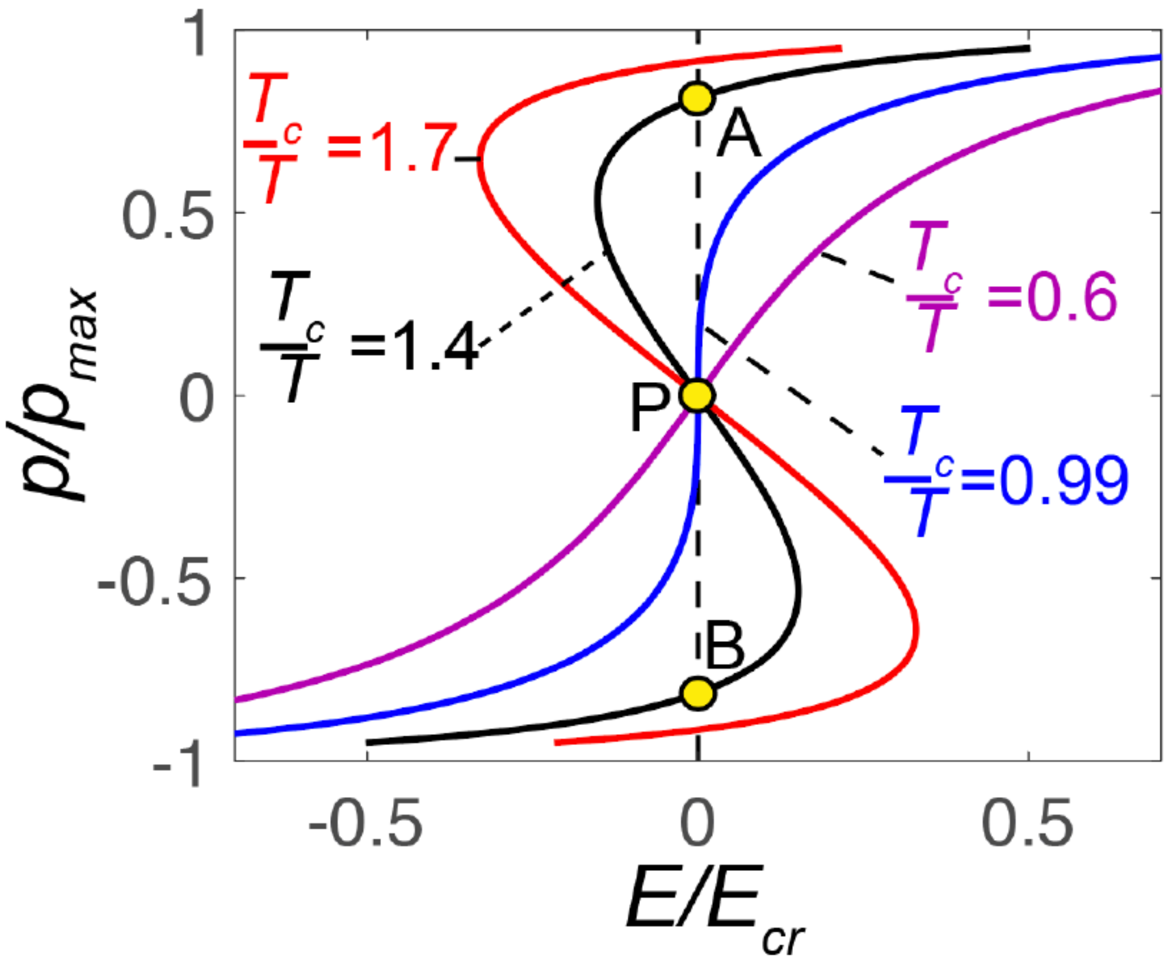
Toy model of Negative Capacitance ('S'-curve)

$$\frac{E}{E_{cr}} = -\frac{T}{T_c}\frac{p}{p_{max}} + \frac{1}{2}\log\frac{1+{}^{p}/_{p_{max}}}{1-{}^{p}/_{p_{max}}}$$



Toy model of Negative Capacitance ('S'-curve)

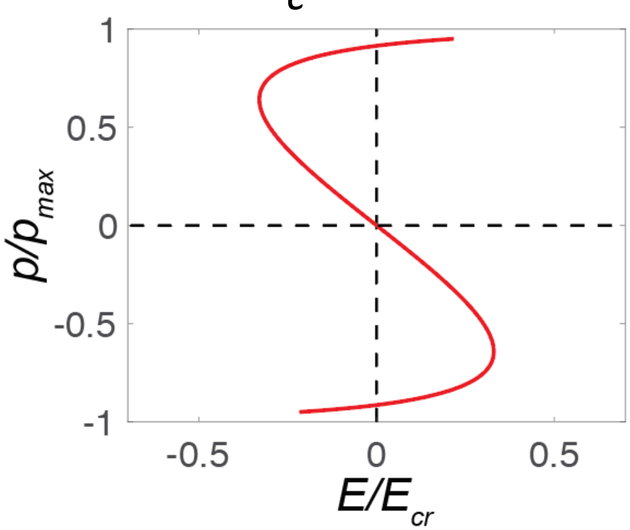
$$\frac{E}{E_{cr}} = -\frac{T}{T_c}\frac{p}{p_{max}} + \frac{1}{2}\log\frac{1 + {}^{p}/_{p_{max}}}{1 - {}^{p}/_{p_{max}}}$$

Maximum moment: $p_{max} = \alpha\epsilon_0 E_{cr}$

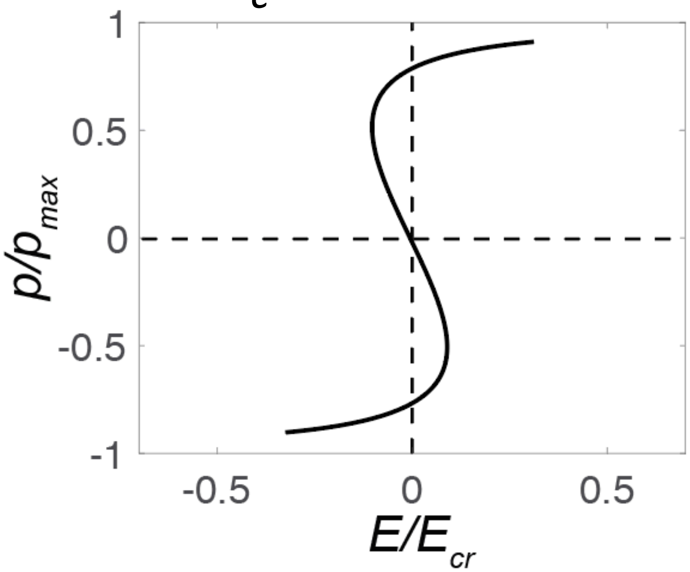
Critical field: E_{cr}

$$\alpha = \frac{1}{\gamma\epsilon_0 \underbrace{T}_{\text{Temperature}}} \qquad \zeta = \gamma \underbrace{T_C}_{\text{Curie Temperature}}$$

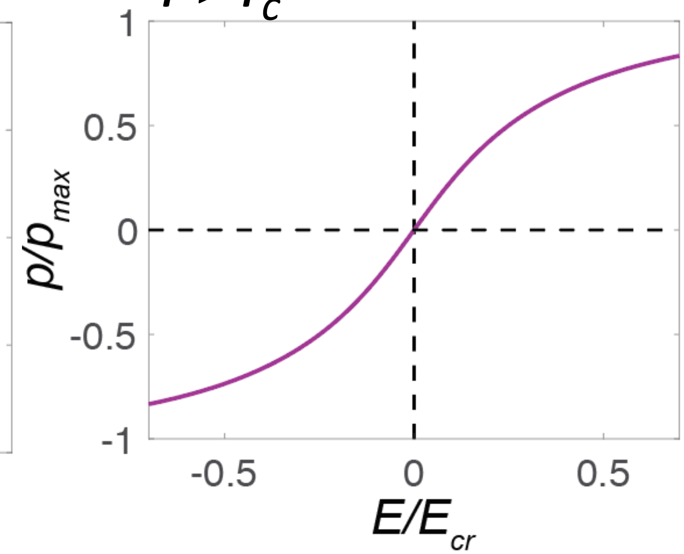
$T << T_c$



$T < T_c$



$T > T_c$



Toy model of Negative Capacitance ('S'-curve)

$$\frac{E}{E_{cr}} = -\frac{T}{T_c}\frac{p}{p_{max}} + \frac{1}{2}\log\frac{1 + {}^{p}/_{p_{max}}}{1 - {}^{p}/_{p_{max}}}$$

$$\Downarrow ?$$

How to get to the Landau expression?

$$E = \alpha_1 P + \alpha_{11} P^3 + \alpha_{111} P^5 + \cdots$$

Toy model of Negative Capacitance (‘S’-curve)

$$\frac{E}{E_{cr}} = -\frac{T}{T_c}\frac{p}{p_{max}} + \frac{1}{2}\log\frac{1 + {}^{p}/_{p_{max}}}{1 - {}^{p}/_{p_{max}}}$$

$$\Downarrow \qquad \log\frac{1+x}{1-x} = x + \frac{x^3}{3} + \frac{x^5}{5} + \cdots$$

$$E = \left(\frac{E_{cr}}{p_{max}} - \zeta\right) p + \frac{E_{cr}}{3{p_{max}}^3} p^3 + \frac{E_{cr}}{5{p_{max}}^5} p^5 + \cdots$$

$$\alpha = \frac{1}{\gamma \epsilon_0 T}$$

$$\zeta = \gamma T_C$$

$$\alpha_1 = \frac{E_{cr}}{p_{max}} - \zeta = {}^{1}/_{\alpha\epsilon_0} - \zeta = \varsigma(T - T_C),$$

$$\alpha_{11} = {}^{E_{cr}}/_{3p_{max}^3}, \; \alpha_{111} = {}^{E_{cr}}/_{5p_{max}^5}$$

$$\Downarrow$$

$$E = \alpha_1 p + \alpha_{11} p^3 + \alpha_{111} p^5 + \cdots$$

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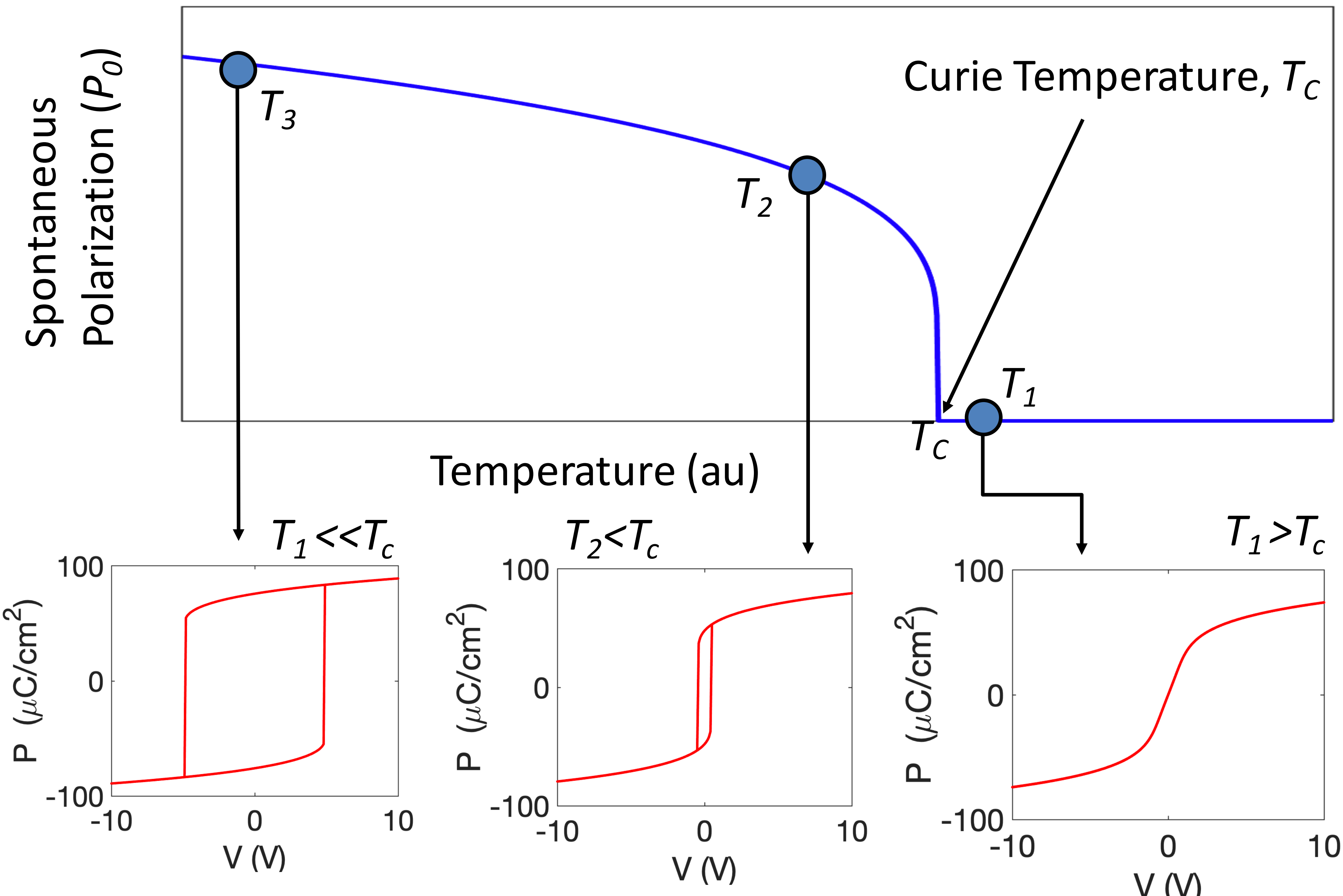
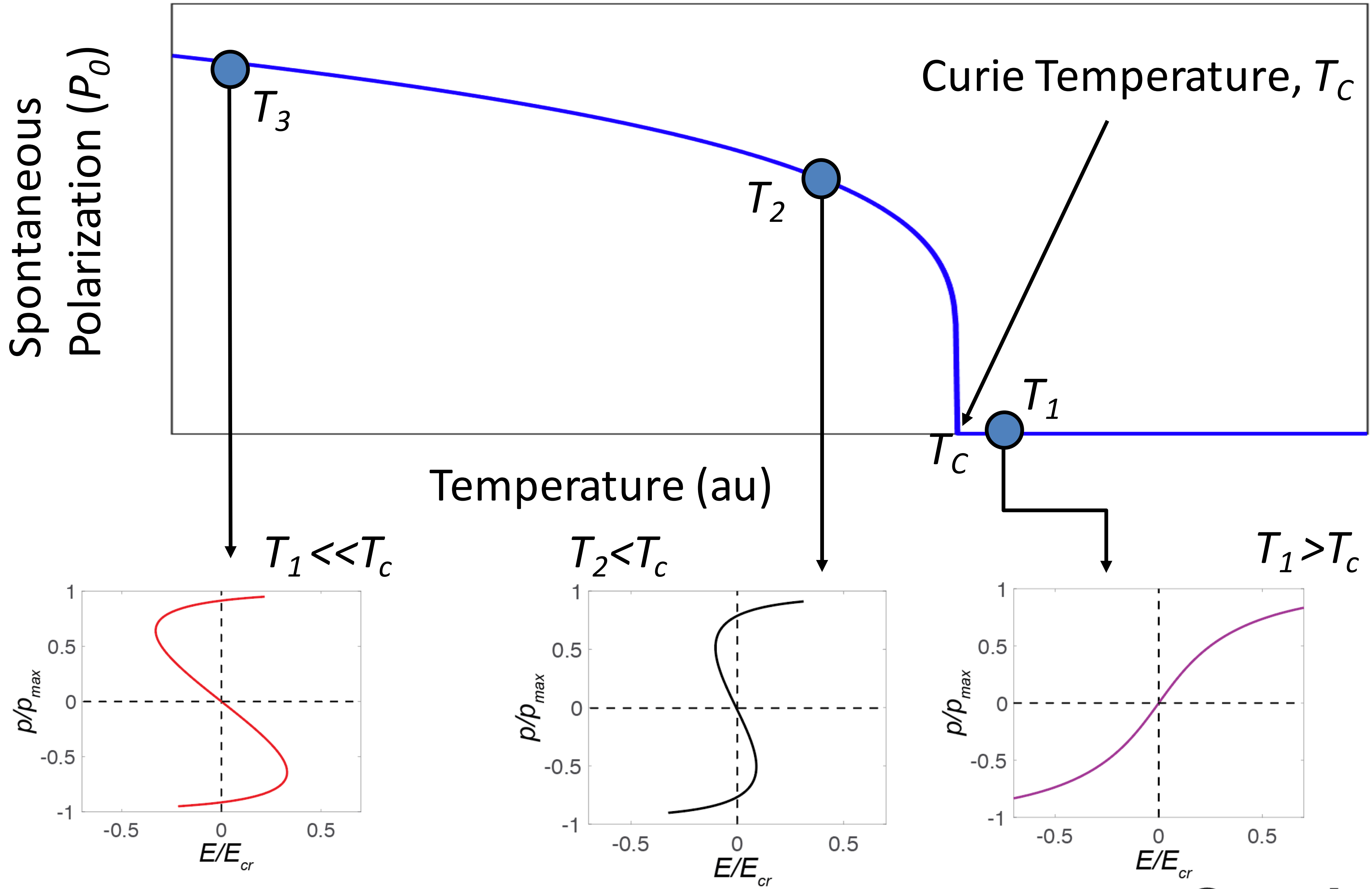
Ferroelectric Oxides: Temperature dependence



Ferroelectric Oxides: Temperature dependence



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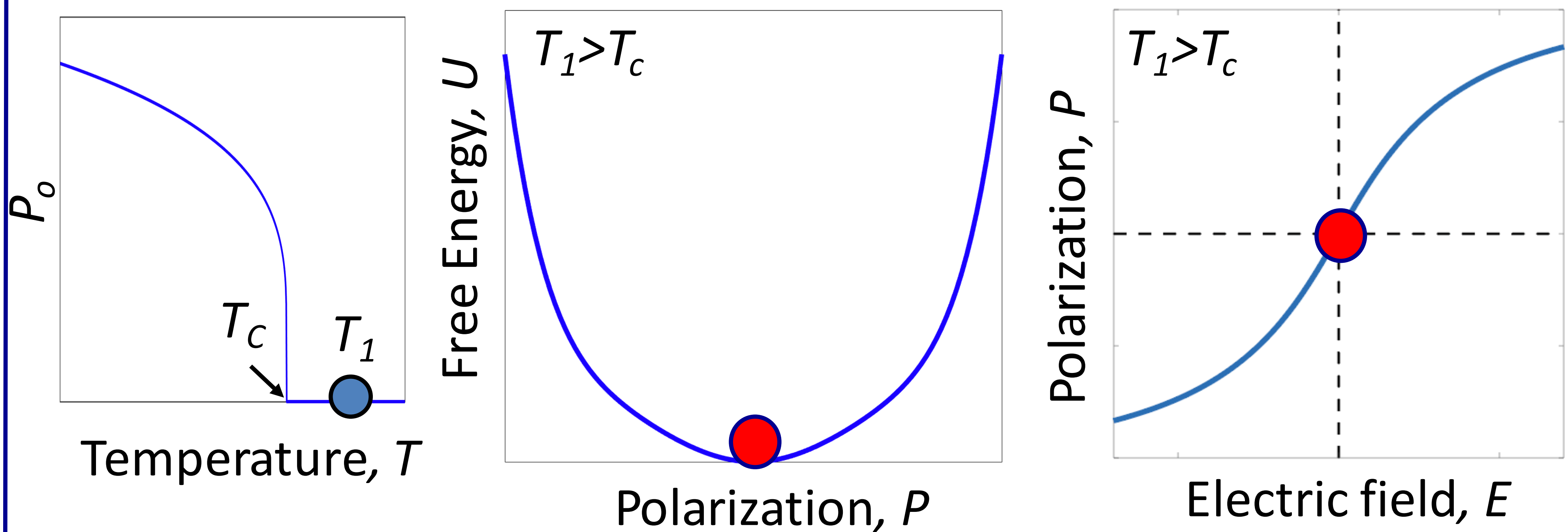
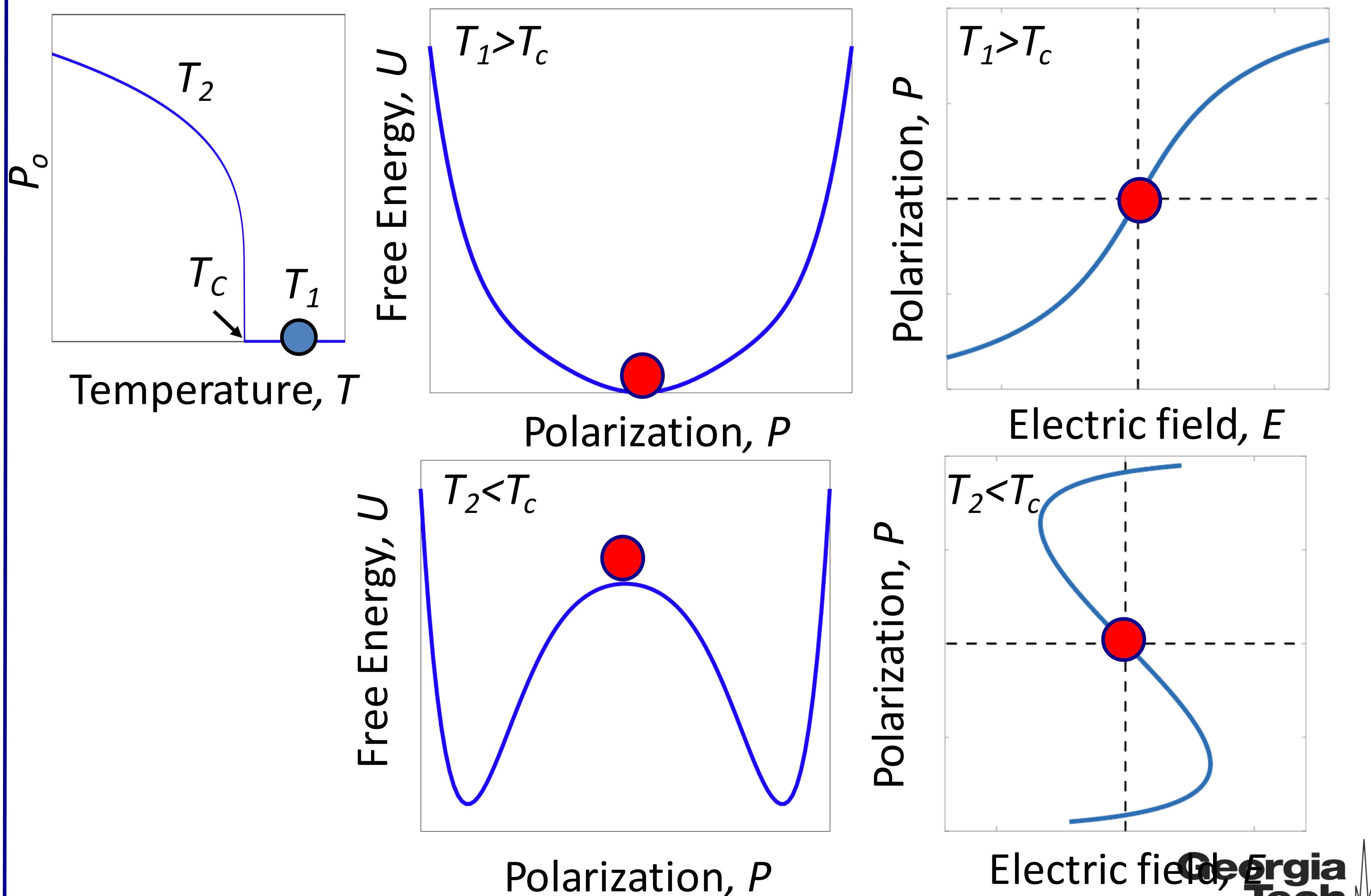
Ferroelectric Oxides: Temperature dependence



<u>A thought experiment:</u>

What happens if we could change temperature extremely fast?

Ferroelectric Oxides: Temperature dependence



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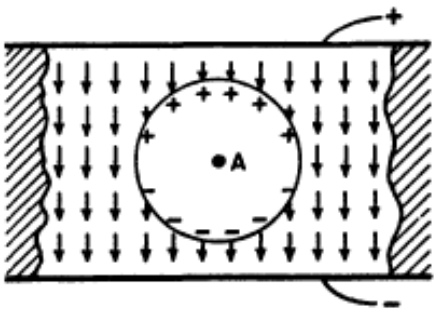
Similar treatment: Clausius-Mossotti Equation

The Clausius Mossoti Picture



$$E_{local} = E_{applied} + E_{Lorentz} + E_{cavity}$$

$$E_{Lorentz} = P_0 / 3\varepsilon_0 , E_{cavity} = 0$$

$$E_{local} = E_{applied} + \frac{P}{3\varepsilon_0}$$

$$P = N\alpha E_{local}$$

E_{local}=Local electric field, $E_{applied}$=Applied electric field, $E_{Lorentz}$=Lorentz cavity Field, E_{cavity}=E-field due to dipoles in the cavity, α = Electronic polarizability, N = Dipole density

Clausius-Mossotti Equation

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha}{3\epsilon_0}$$

$$\chi = \varepsilon_r - 1 = \frac{N\alpha / \varepsilon_0}{1 - N\alpha / \varepsilon_0} < 0$$

if $N\alpha / 3\varepsilon_0 > 1$

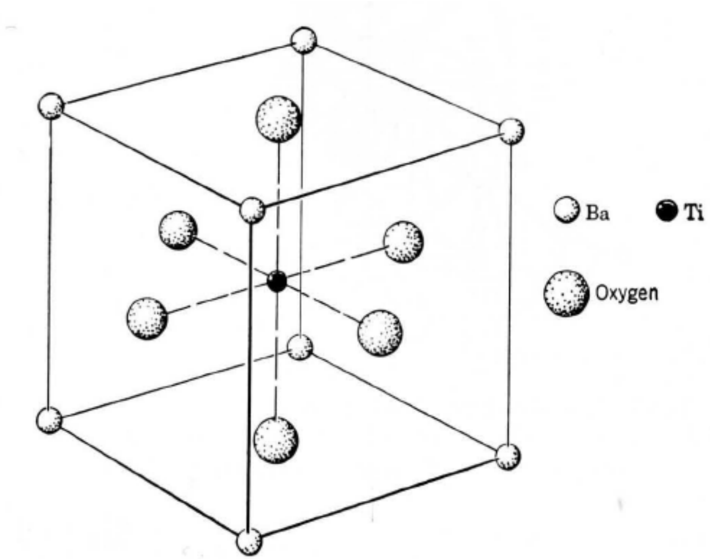
Clausius-Mossotti equation is often used to describe polar dielectrics. [Kittel: Introduction to Solid State Physics]

Similar treatments of Ferroelectric

PHYSICAL REVIEW VOLUME 78, NUMBER 6 JUNE 15, 1950

The Lorentz Correction in Barium Titanate

J. C. Slater
*Massachusetts Institute of Technology, Cambridge, Massachusetts**
(Received March 13, 1950)



$$\begin{aligned}
E(\mathrm{Ba}) &= P(\mathrm{Ba})/N(\mathrm{Ba})\alpha(\mathrm{Ba}) \\
&= E_0 + q_{11}P(\mathrm{Ba}) + q_{12}P(\mathrm{Ti}) + q_{13}P(\mathrm{O}') + q_{14}P(\mathrm{O}''); \\
E(\mathrm{Ti}) &= P(\mathrm{Ti})/N(\mathrm{Ti})\alpha(\mathrm{Ti}) \\
&= E_0 + q_{21}P(\mathrm{Ba}) + q_{22}(\mathrm{Ti}) + q_{23}P(\mathrm{O}') + q_{24}P(\mathrm{O}''); \\
E(\mathrm{O}') &= P(\mathrm{O}')/N(\mathrm{O}')\alpha(\mathrm{O}') \\
&= E_0 + q_{31}P(\mathrm{Ba}) + q_{32}P(\mathrm{Ti}) + q_{33}P(\mathrm{O}') + q_{34}P(\mathrm{O}''); \\
E(\mathrm{O}'') &= P(\mathrm{O}'')/N(\mathrm{O}'')\alpha(\mathrm{O}'') \\
&= E_0 + q_{41}P(\mathrm{Ba}) + q_{42}P(\mathrm{Ti}) + q_{43}P(\mathrm{O}') + q_{44}P(\mathrm{O}'').
\end{aligned}$$

$$\begin{aligned}
\alpha(\mathrm{Ba}) &= 1.95 \times 10^{-24}\ \mathrm{cm}^3, \\
\alpha(\mathrm{O}') &= \alpha(\mathrm{O}'') = 2.4 \times 10^{-24}\ \mathrm{cm}^3, \\
\alpha(\mathrm{Ti}) &= 0.19 \times 10^{-24} + \alpha_i(\mathrm{Ti});
\end{aligned}$$

$$\epsilon \approx \frac{3T_c}{T - T_c}$$

$$\begin{aligned}
\alpha_i(\mathrm{Ti}) &= 0.95 \times 10^{-24}\ \mathrm{cm}^3, \\
(4\pi/3)N(\mathrm{Ti})\alpha_i(\mathrm{Ti}) &= 0.062,
\end{aligned}$$

Similar treatment was done in 1950s.

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Is a negative capacitance is a <u>real, physical phenomenon</u> or an <u>unphysical, artificial construct</u> of the phenomenology of the Landau Theory?

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DRC 2019, June 24, 2019

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Negative capacitance is a real….

physical phenomenon!

Arises from simple dipole-dipole interactions and positive feedback mechanisms!

Without negative capacitance (i.e., static negative dielectric permittivity), ferroelectrics do not exist!

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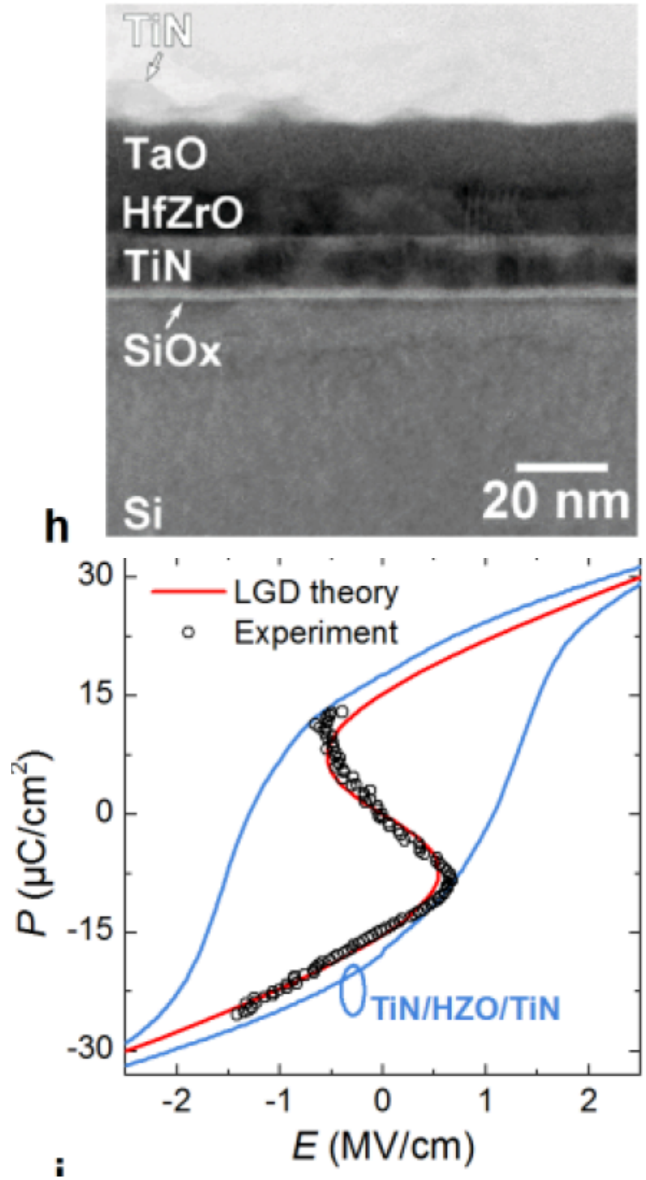
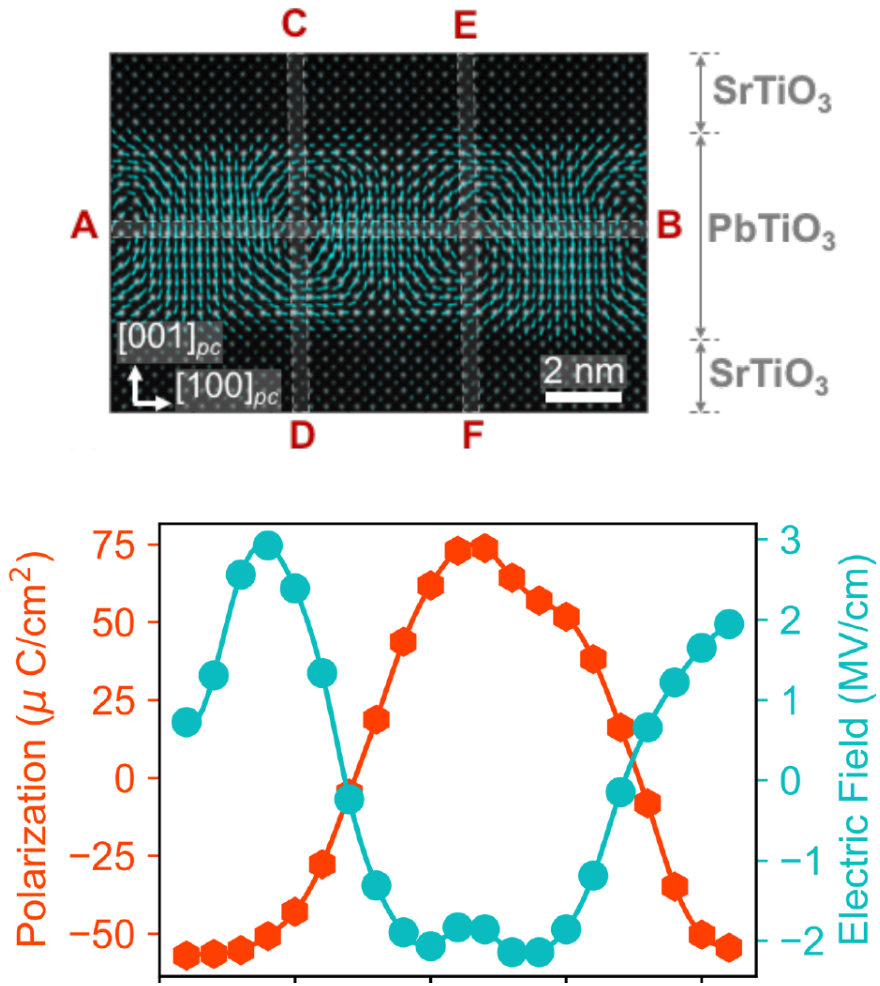
Experimentally Measured ‘S’-curve

Hoffmann et al. Nature 2018

Hoffmann et al. IEDM 2018 p. 31.6

Yadav et al. 2018 (in press)





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Microscopic Origin of Negative Capacitance in Ferroelectrics

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Thanks & Questions

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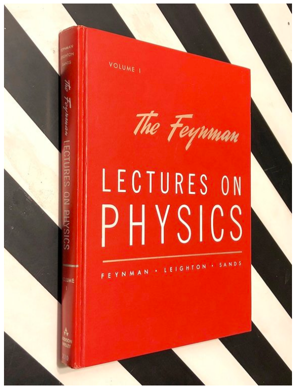
Throw back to Feynman



Feynman Lectures on Physics, vol. 3
Chapter 11

Now when we wrote Eq. (11.28) you may have wondered what would happen if $N\alpha$ became greater than 3. It appears as though κ would become negative. But that surely cannot be right. Let's see what should happen if we were gradually to increase α in a particular crystal. As α gets larger, the polarization gets bigger, making a bigger local field. But a bigger local field will polarize each atom more, raising the local fields still more. If the "give" of the atoms is enough, the process keeps going; there is a kind of feedback that causes the polarization to increase without limit—assuming that the polarization of each atom increases in proportion to the field. The "runaway" condition occurs when $N\alpha = 3$. The polarization does not become infinite, of course, because the proportionality between the induced moment and the electric field breaks down at high fields, so that our formulas are no longer correct. What happens is that the lattice gets "locked in" with a high, self-generated, internal polarization.

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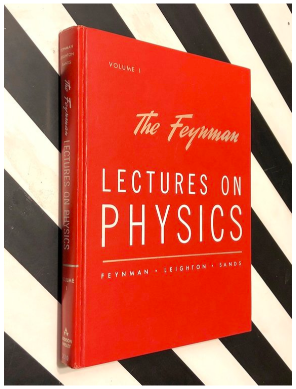
Throw back to Feynman



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