UNIVERSITY OF CAMBRIDGE

IA Materials Science: Course B
Materials for Devices

Bartomeu Monserrat
Course B: Materials for Devices

Professor M does Science

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

Who am I?

Digital lab

quantum mechanics

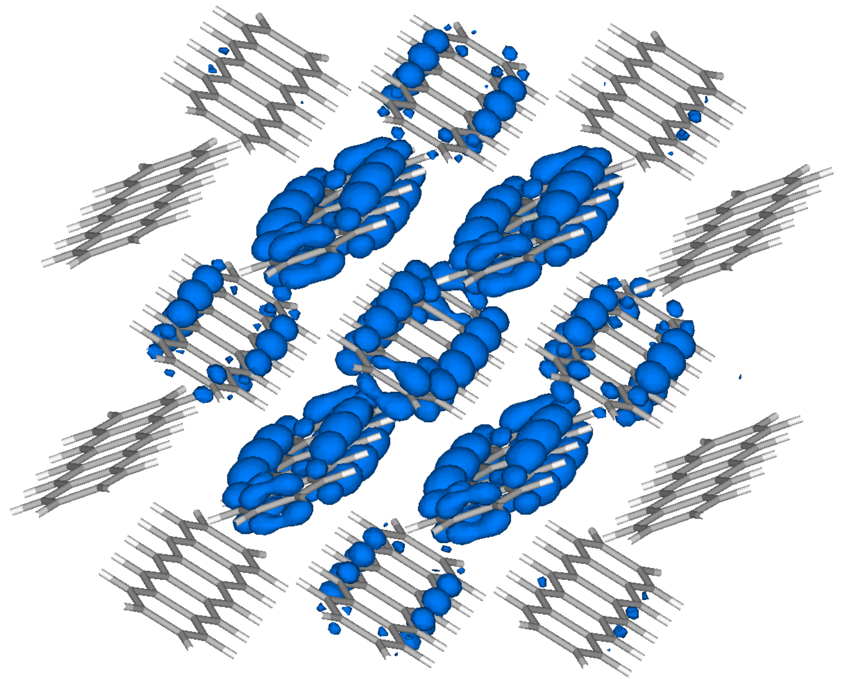
+

machine learning

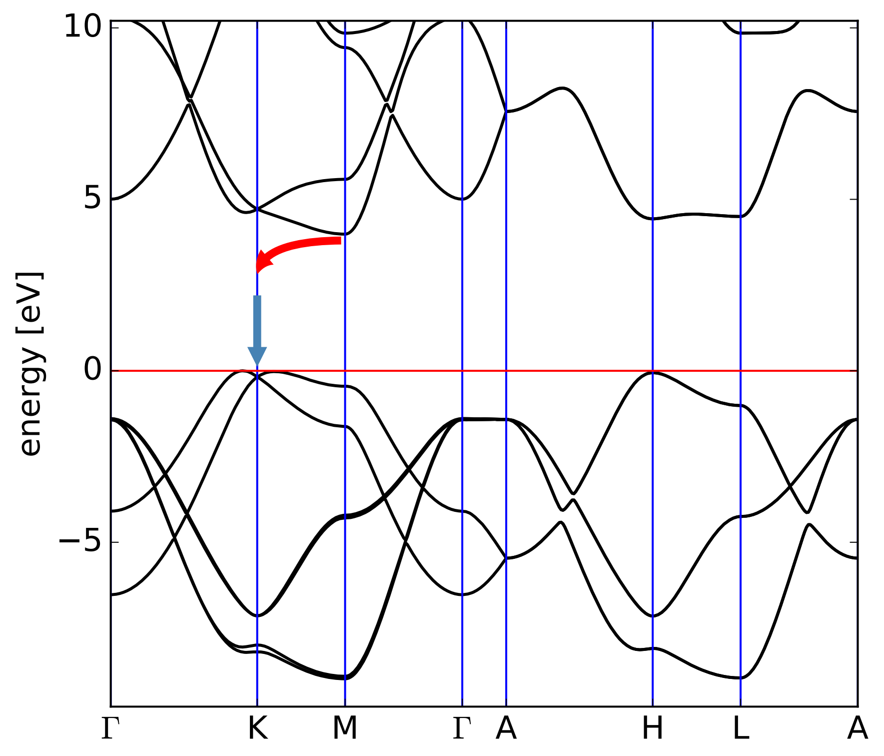
predict and understand material properties

Who am I?

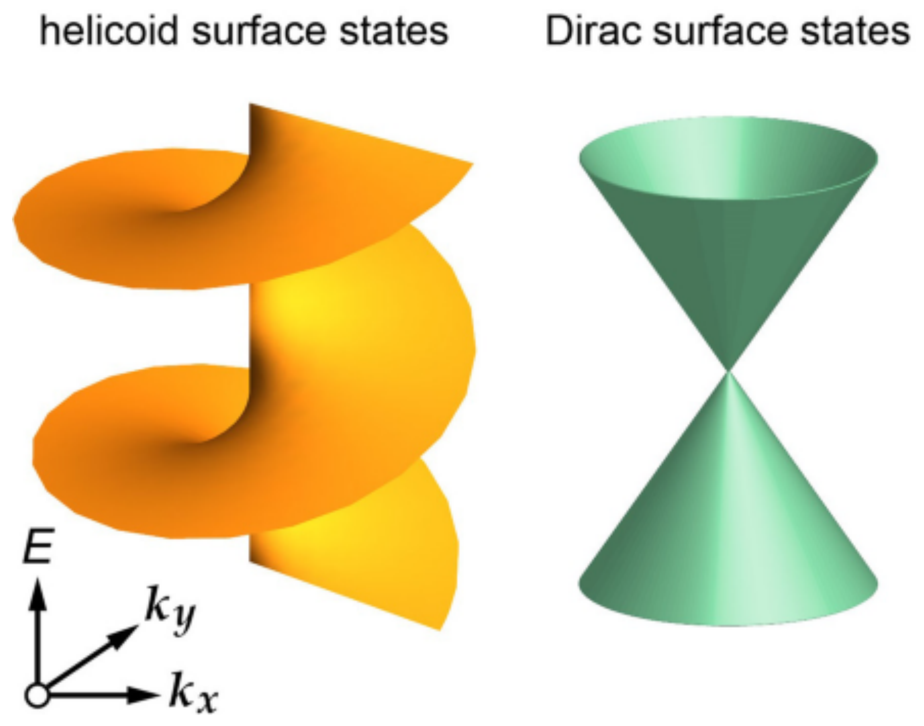
organic semiconductors



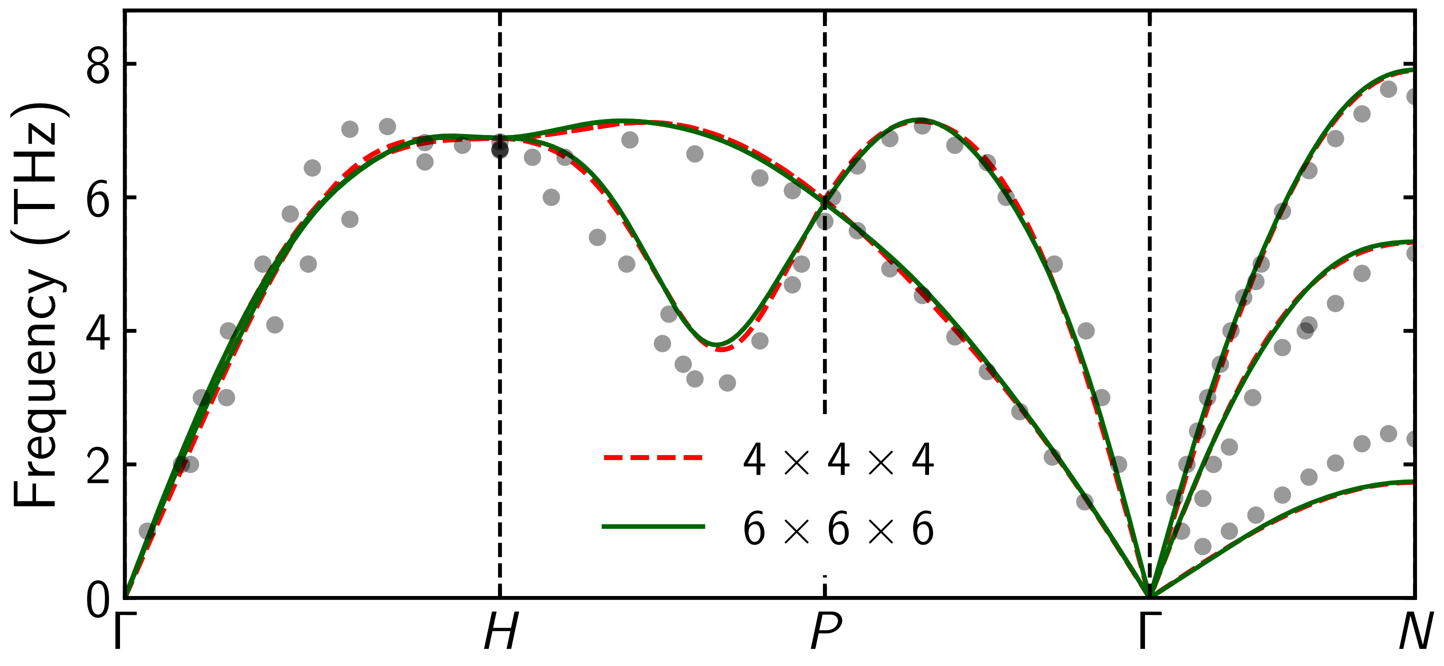
inorganic semiconductors



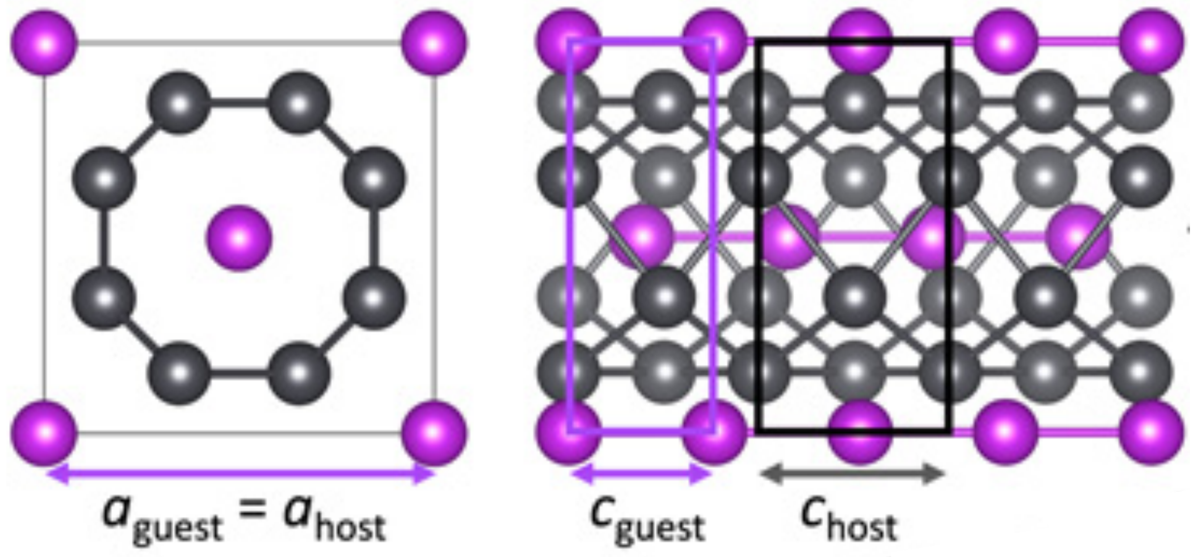
topological insulators and semimetals



magnetic materials



superconductors



Who am I?

Eigenvalues and eigenstates in quantum mechanics

60K views • 4 years ago

The spherical harmonics

58K views • 2 years ago

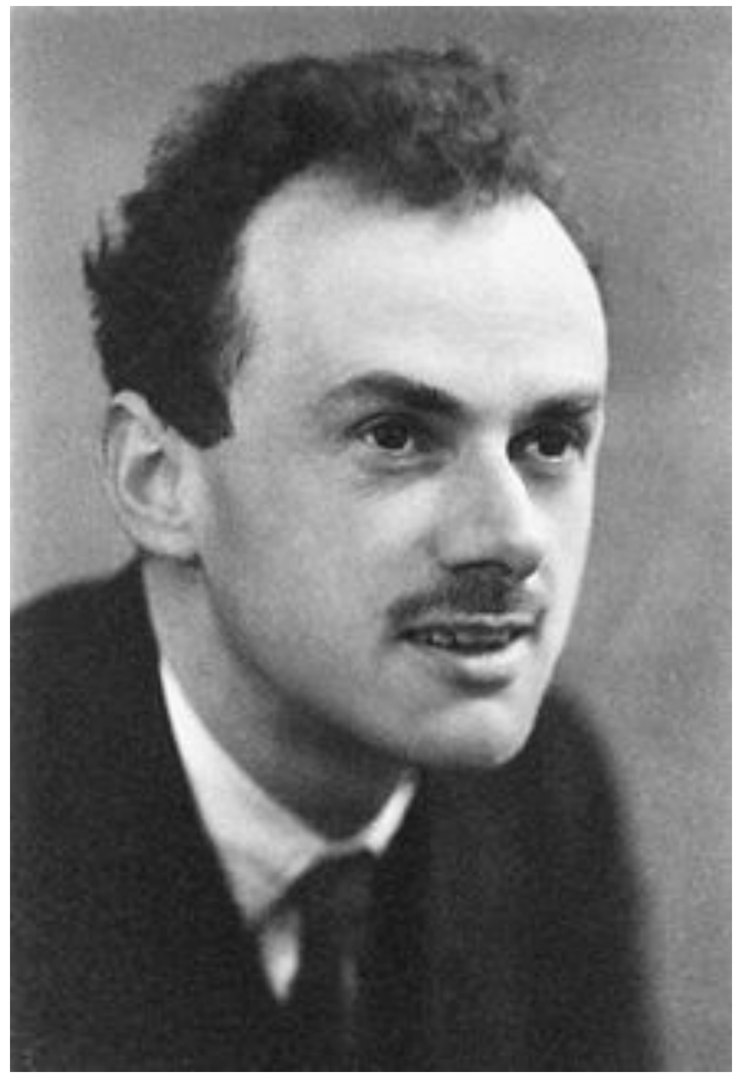
Angular momentum in quantum mechanics

56K views • 3 years ago

The quantum harmonic oscillator

46K views • 3 years ago

What is materials science?



Paul Dirac

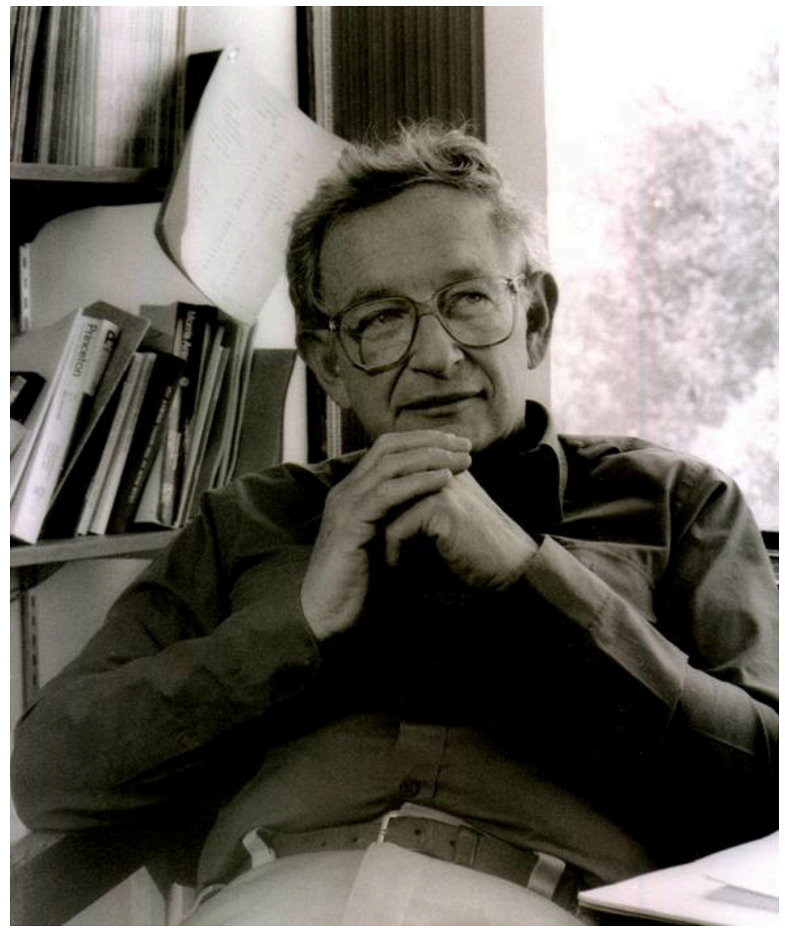
"The underlying physical laws for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation"

Quantum Mechanics of Many-Electron Systems
Proceedings of the Royal Society A 123, 714 (1929)

Nobel Prize in Physics 1933 (together with Schrödinger)

"for the discovery of new productive forms of atomic theory"

What is materials science?



Phil Anderson

"The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behaviour of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear."

More is Different
Science 177, 393 (1972)

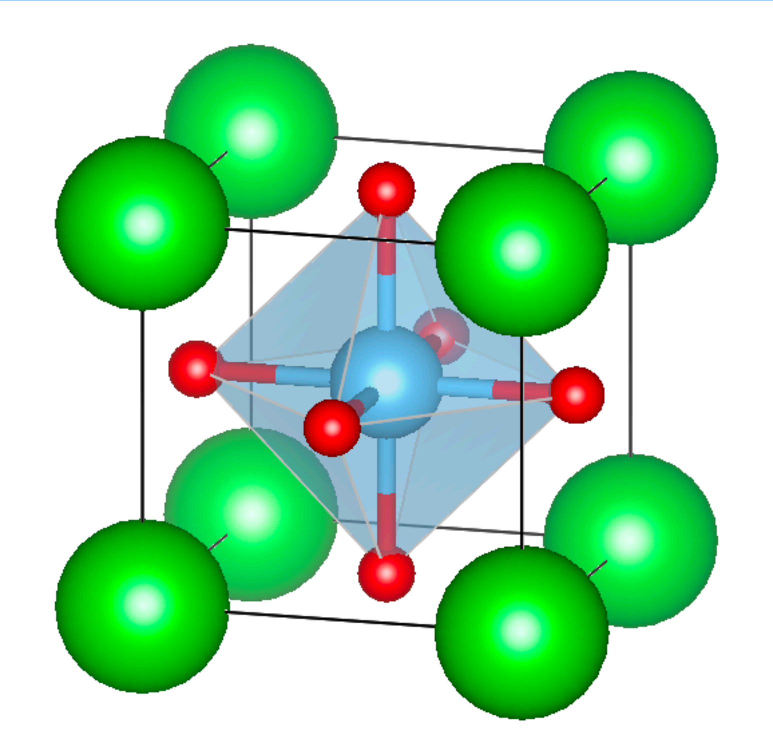
Nobel Prize in Physics 1977 (together with Mott and Van Vleck)

"for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems"

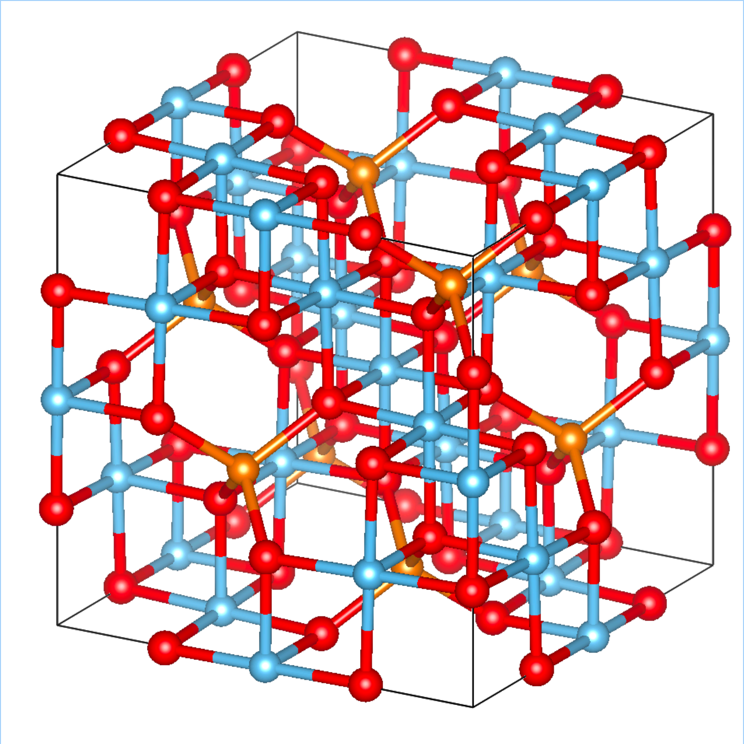
Course B: Materials for Devices

order → disorder

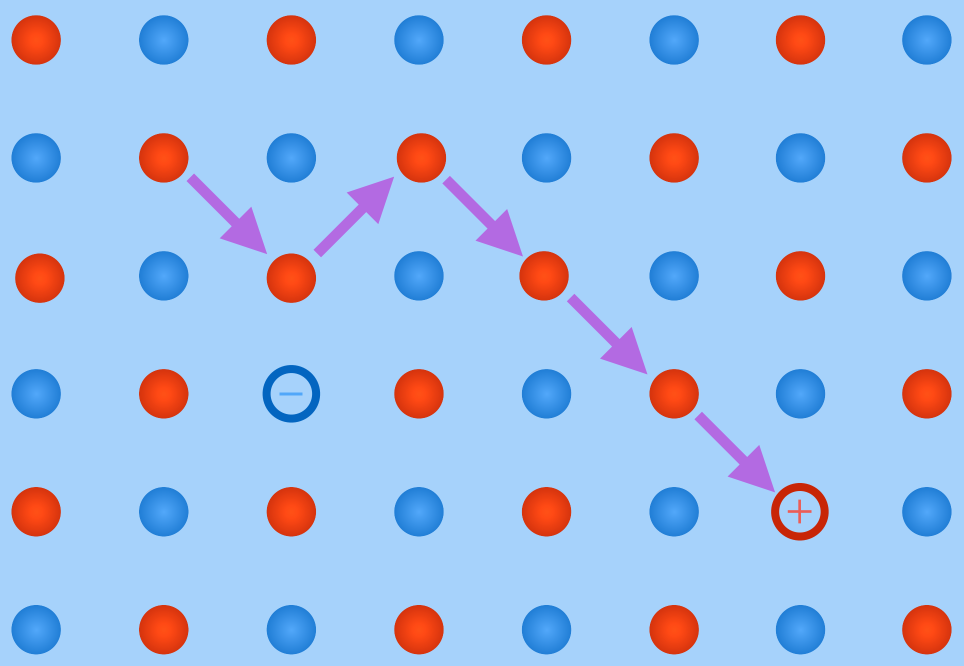
electric polarisation in materials



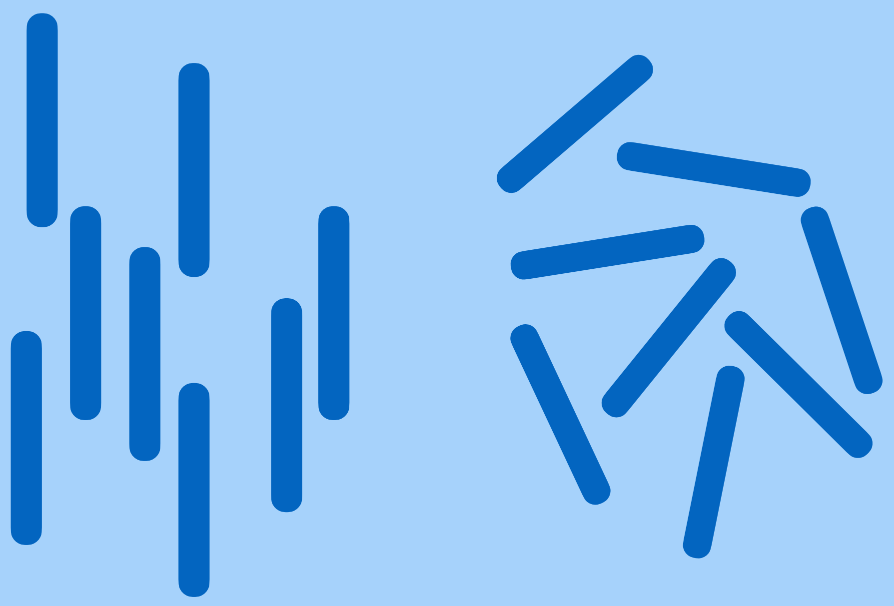
magnetism in materials



ionic conductors



liquid crystals



Course B: Materials for Devices

- **Lectures:**
  - Slides: will be available on Moodle
  - All lectures are recorded and will be available for the rest of the year
  - *Lectures are for understanding the bigger picture*

- **Supervisions and Labs:**
  - Supervisions to go over course material in detail
  - Labs cover some of the topics discussed in lectures
  - *Supervisions and labs are for understanding the details*

- **Resources:**
  - Handout: relatively new, any typos/errors/clarifications welcome!
  - Problems + solutions: check my group website at www.tcm.phy.cam.ac.uk/~bm418/
  - Talk to each other
  - Textbooks and online resources
  - *Other resources are for gaining independence and self-sufficiency*

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Electric polarisation in materials

Lecture 1

Bartomeu Monserrat
Course B: Materials for devices

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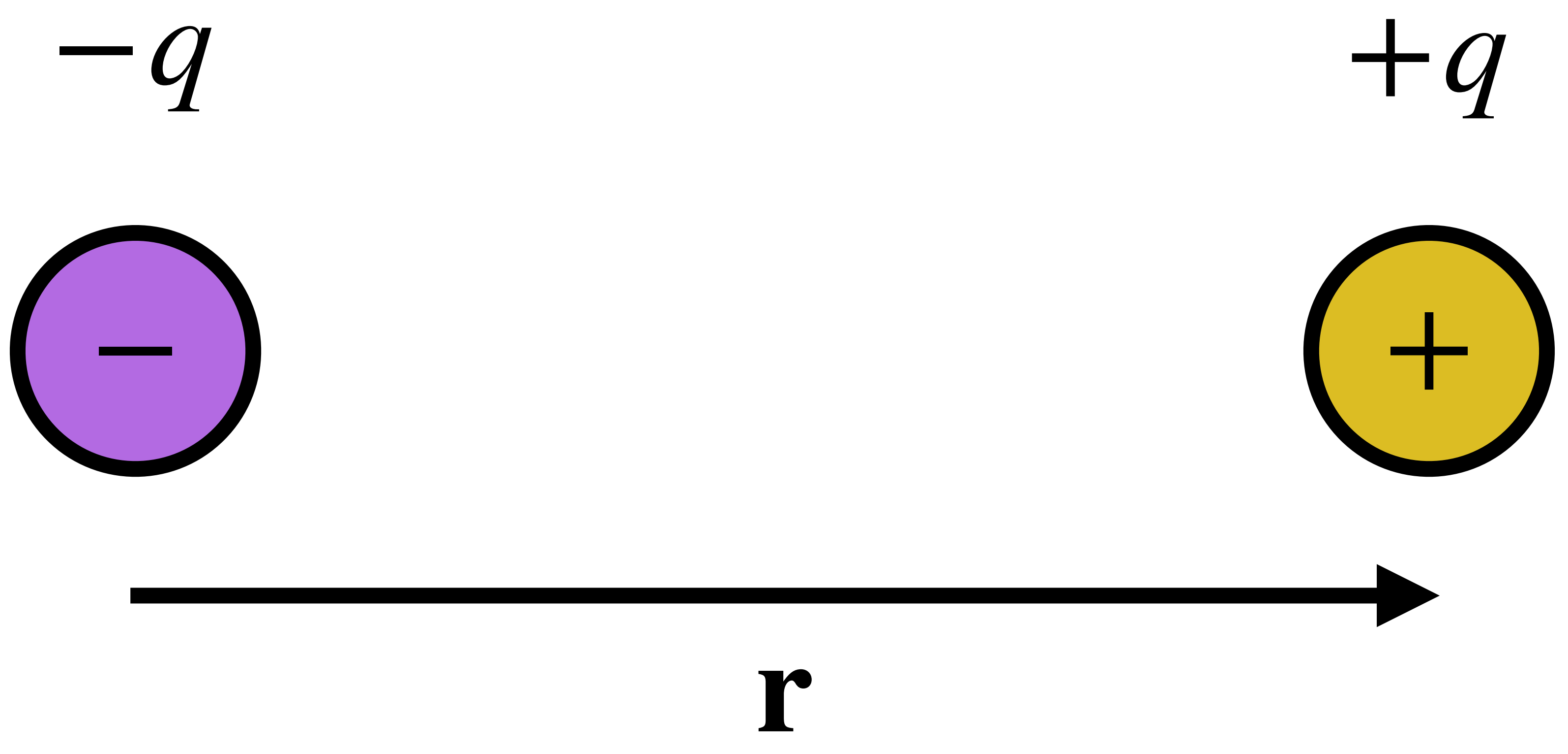
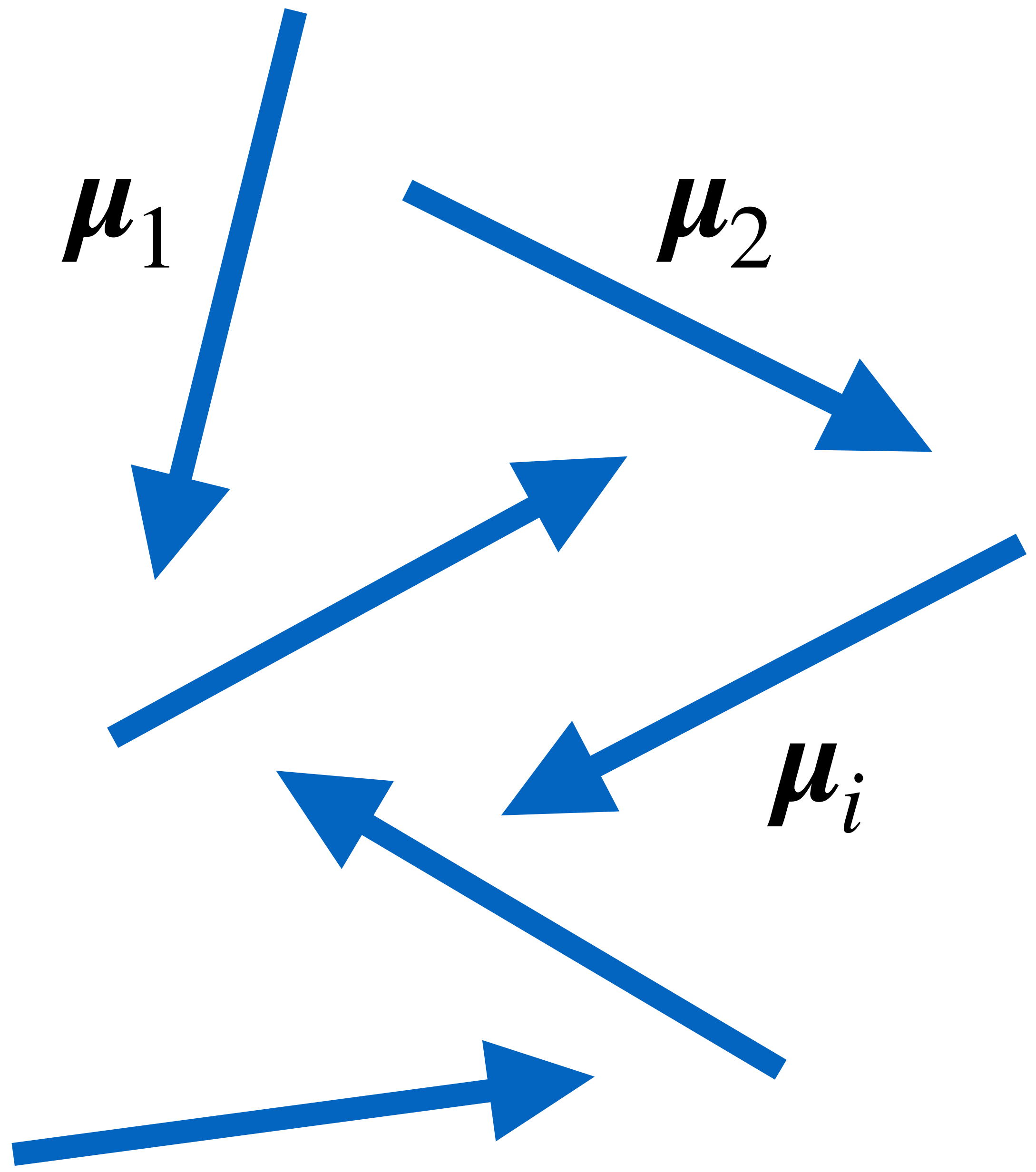
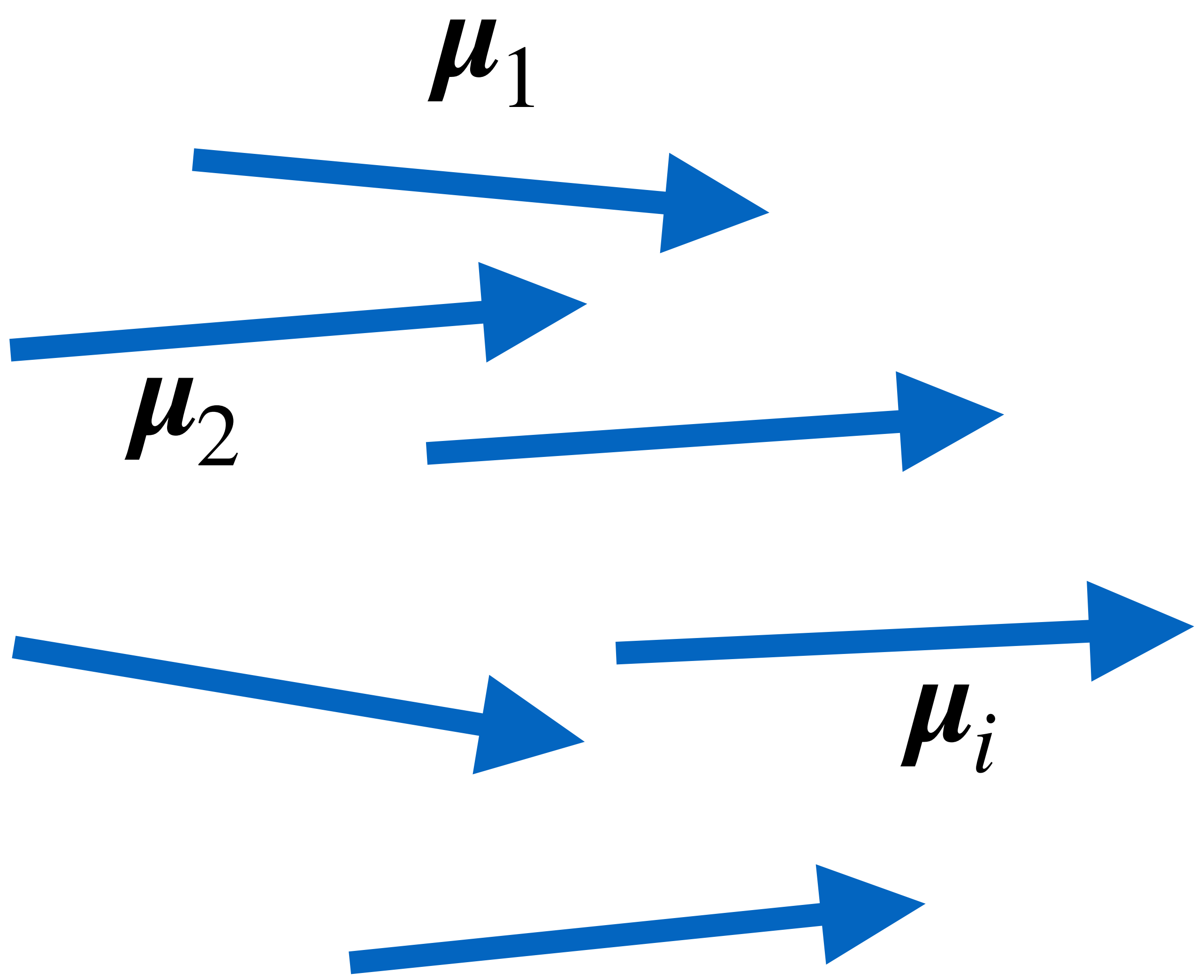
Electric dipole moment



$$\boldsymbol{\mu} = q\mathbf{r} \qquad [\mathrm{C\,m}]$$

Electric dipole moment

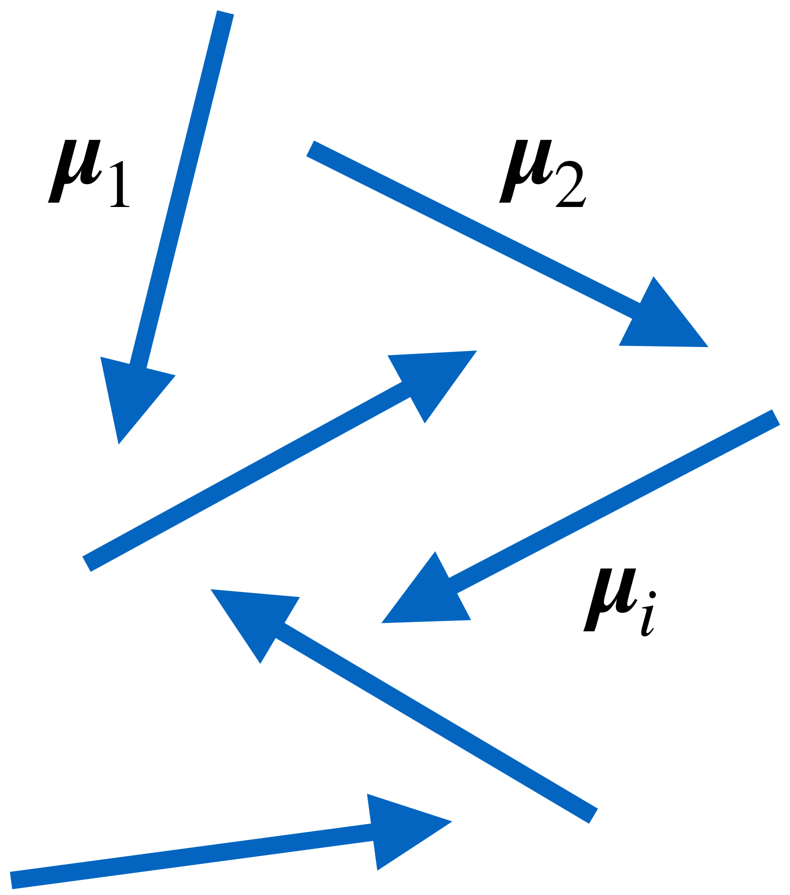


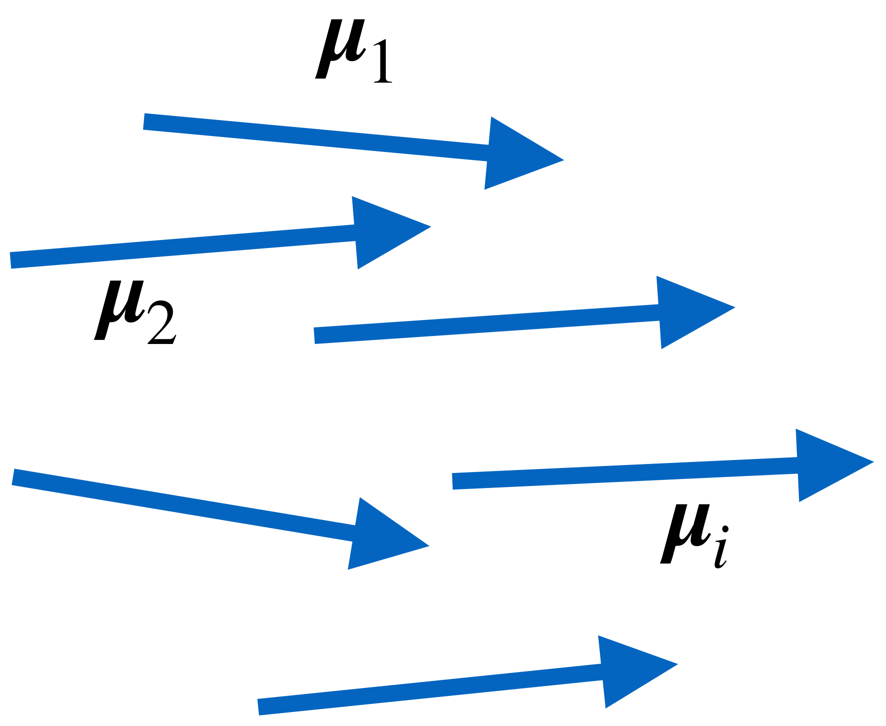


$$\boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq 0$$

$$\boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq N\boldsymbol{\mu}_1$$

Polarisation



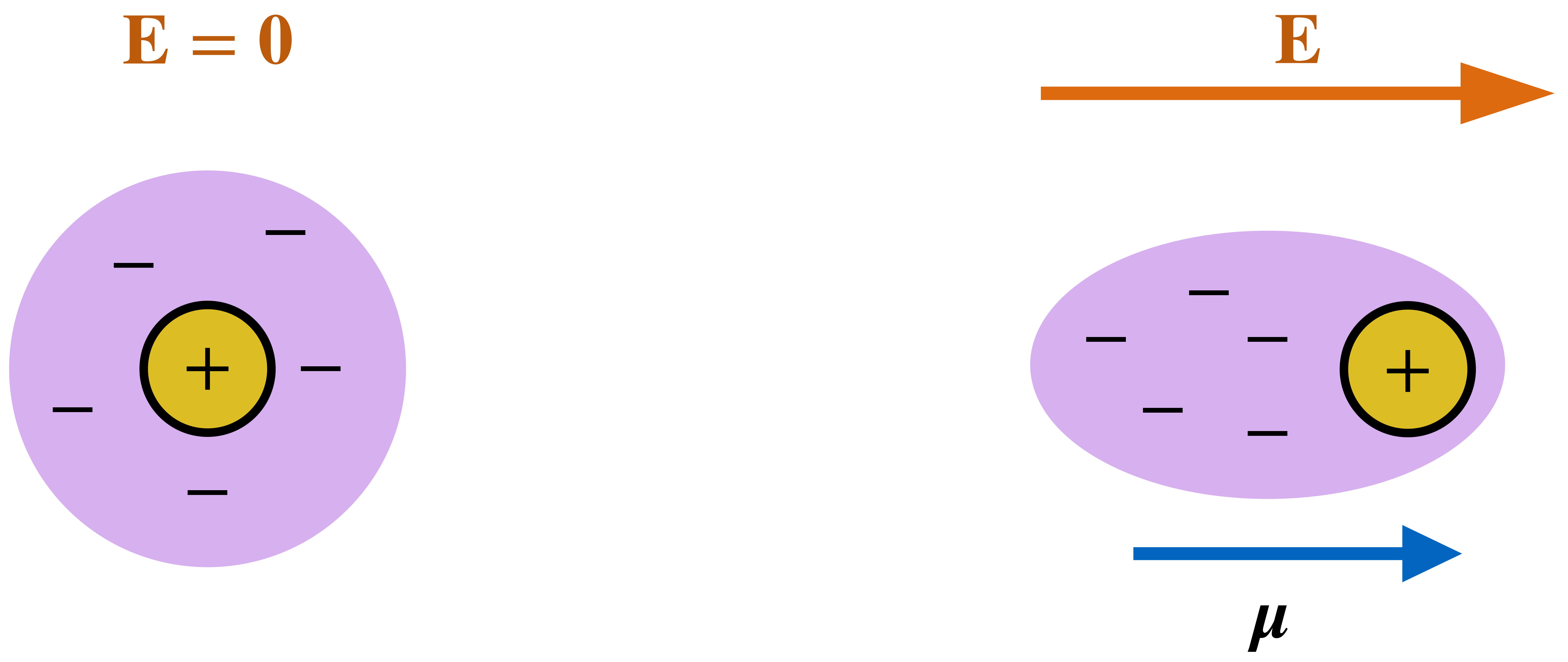


$$\boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq 0 \qquad \boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq N\boldsymbol{\mu}_1$$

$$\boxed{\mathbf{P} = n\boldsymbol{\mu}} \qquad [\mathrm{C\,m^{-2}}]$$

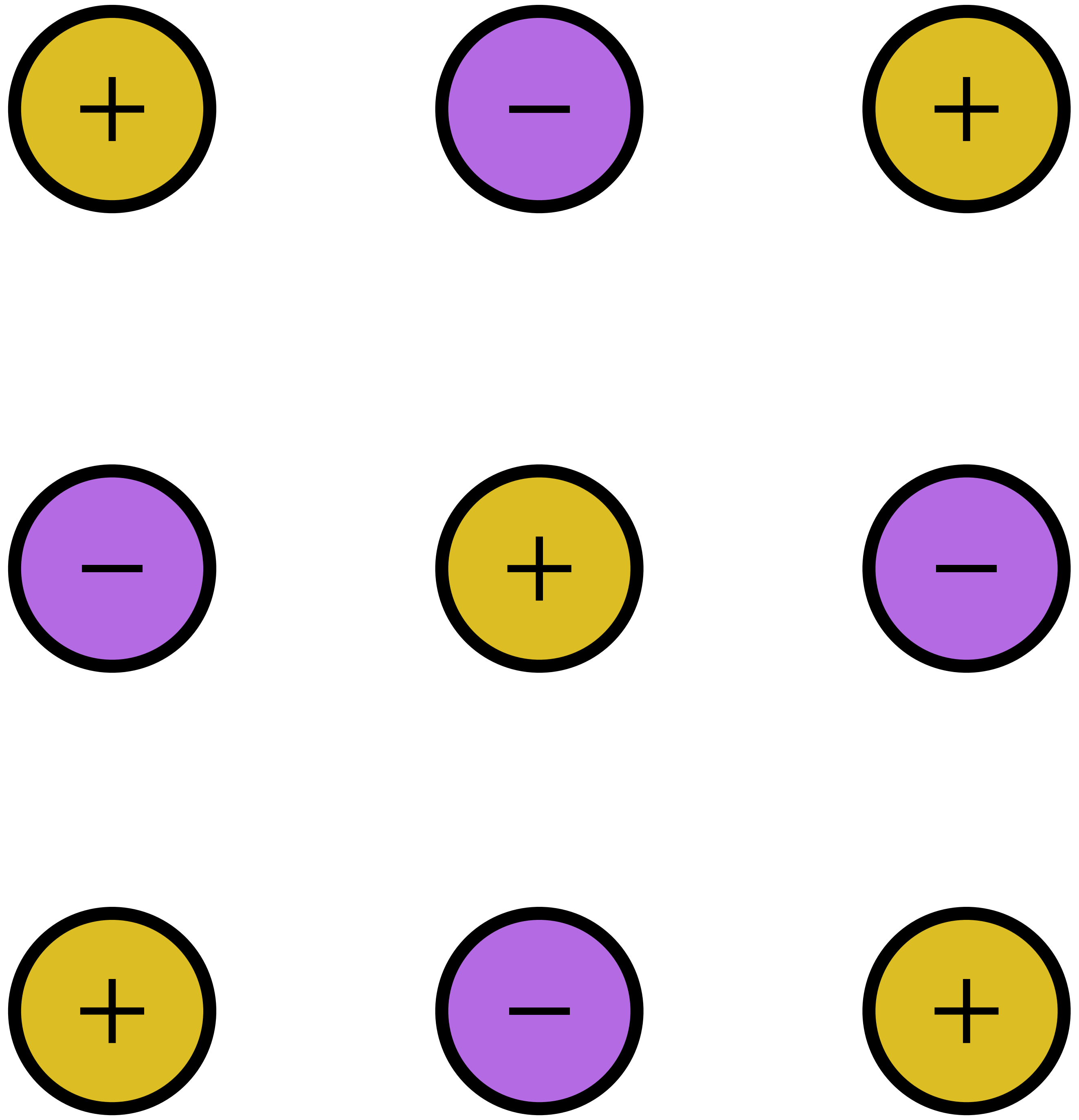
n : number of dipoles per unit volume $[\mathrm{m^{-3}}]$

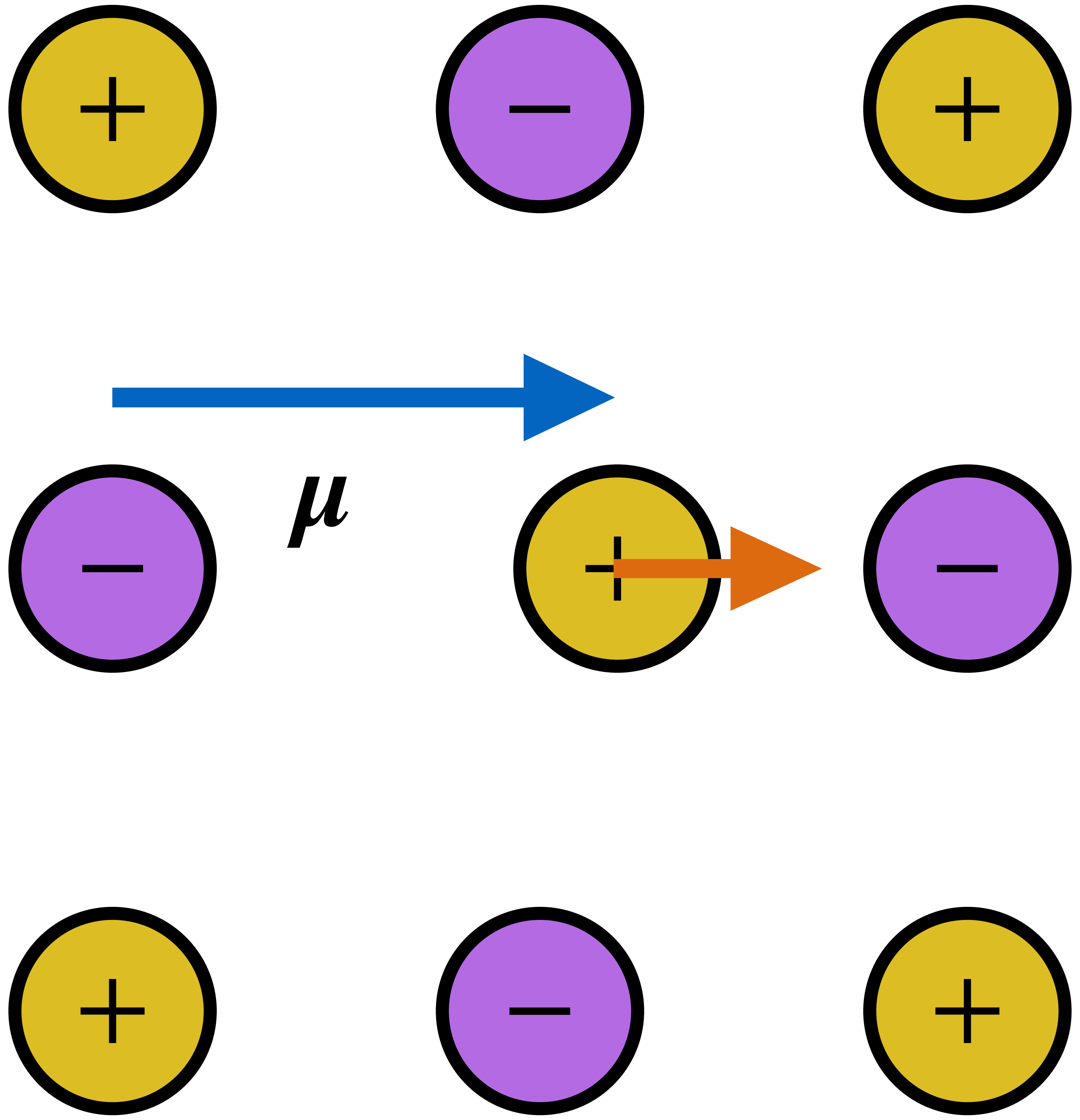
Polarisation mechanisms: electronic polarisation



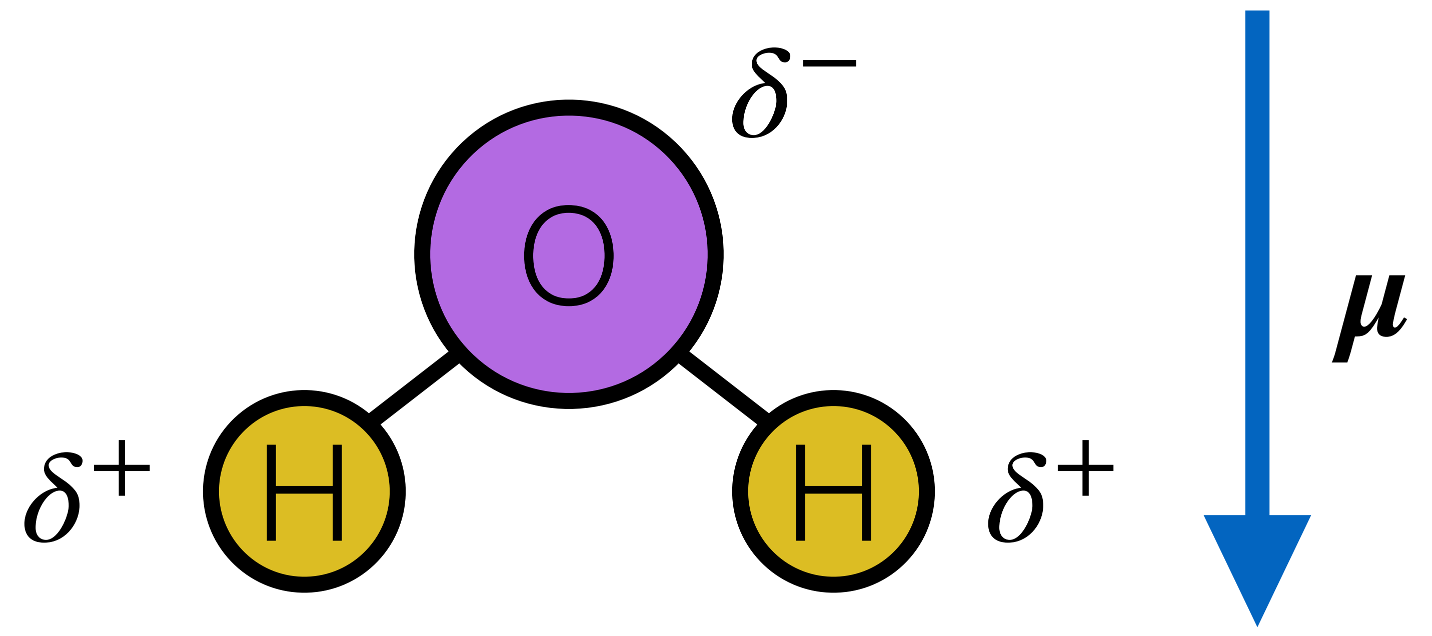
Polarisation mechanisms: ionic polarisation

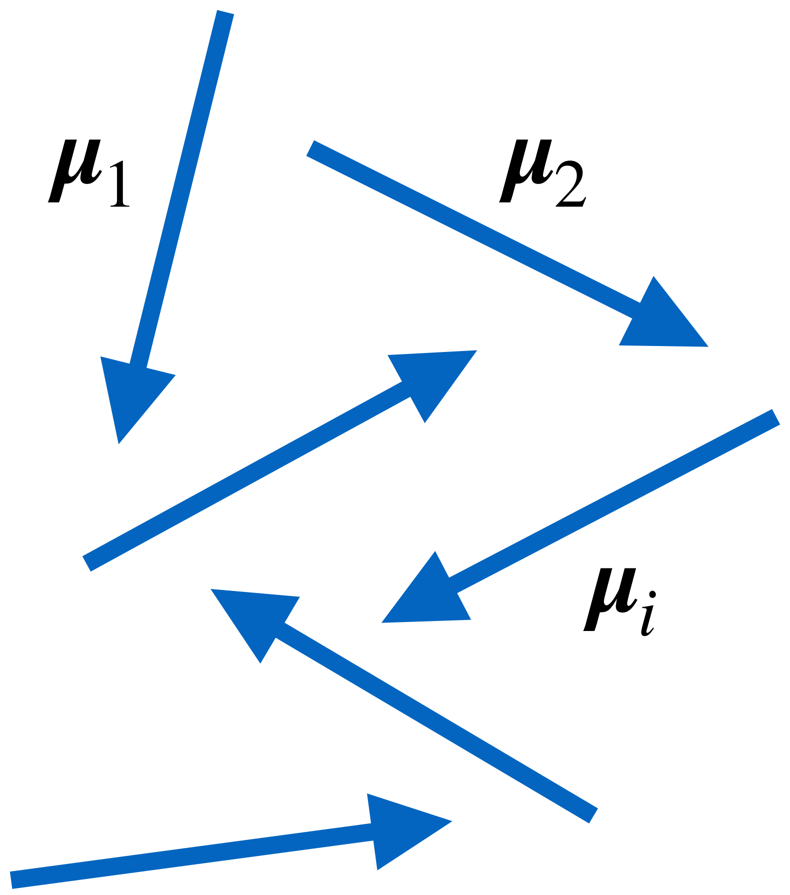
$\mu = 0$



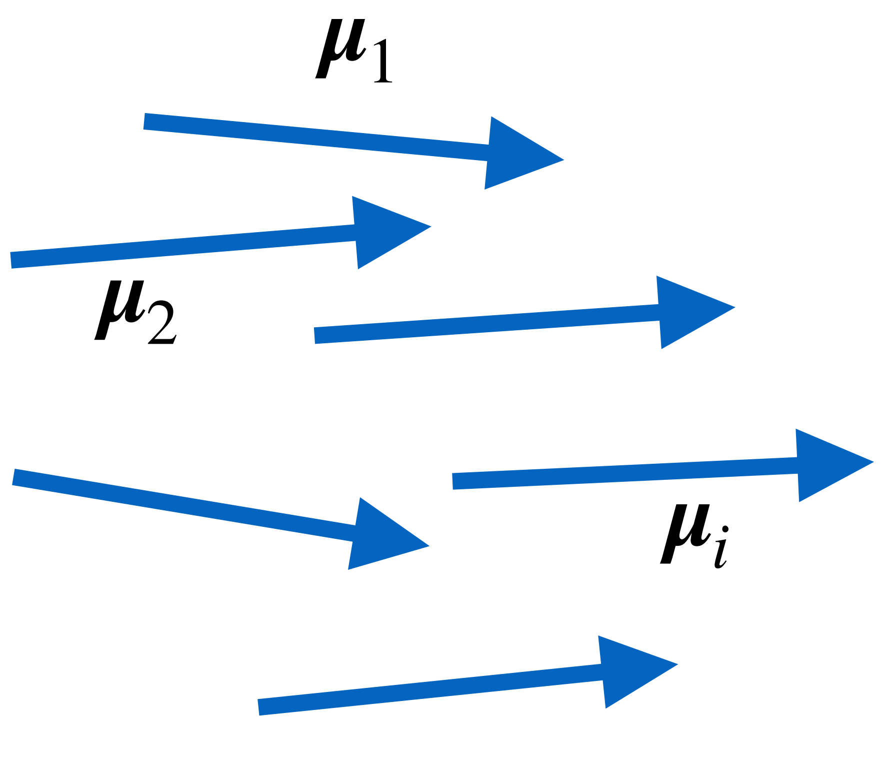


Polarisation mechanisms: orientation (molecular) polarisation





$$\boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq 0$$



$$\boldsymbol{\mu} = \sum_{i=1}^{N} \boldsymbol{\mu}_i \simeq N\boldsymbol{\mu}_1$$

Dielectric materials

- Dielectric material: electrical insulator that can be polarised by applied electric field

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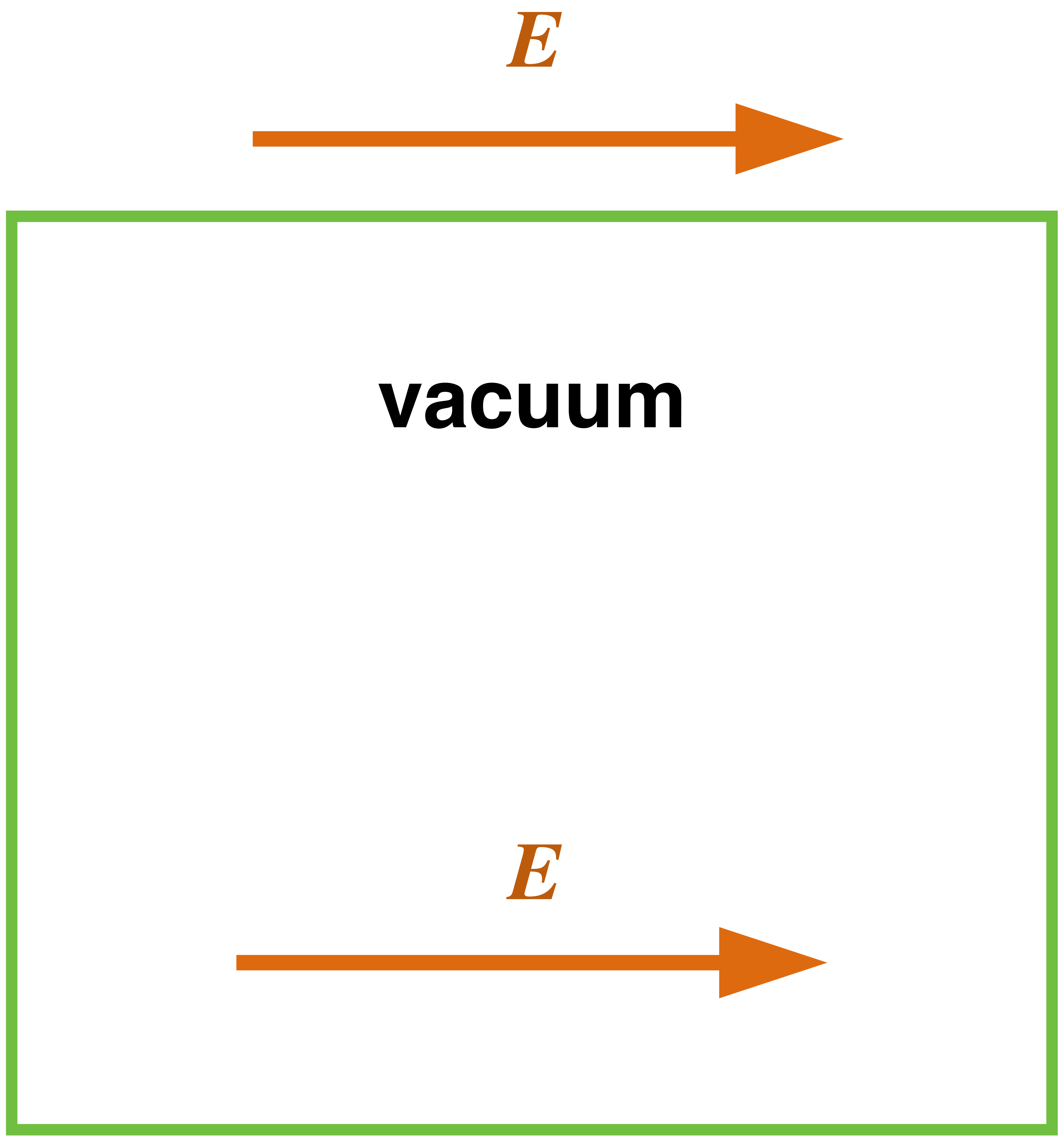
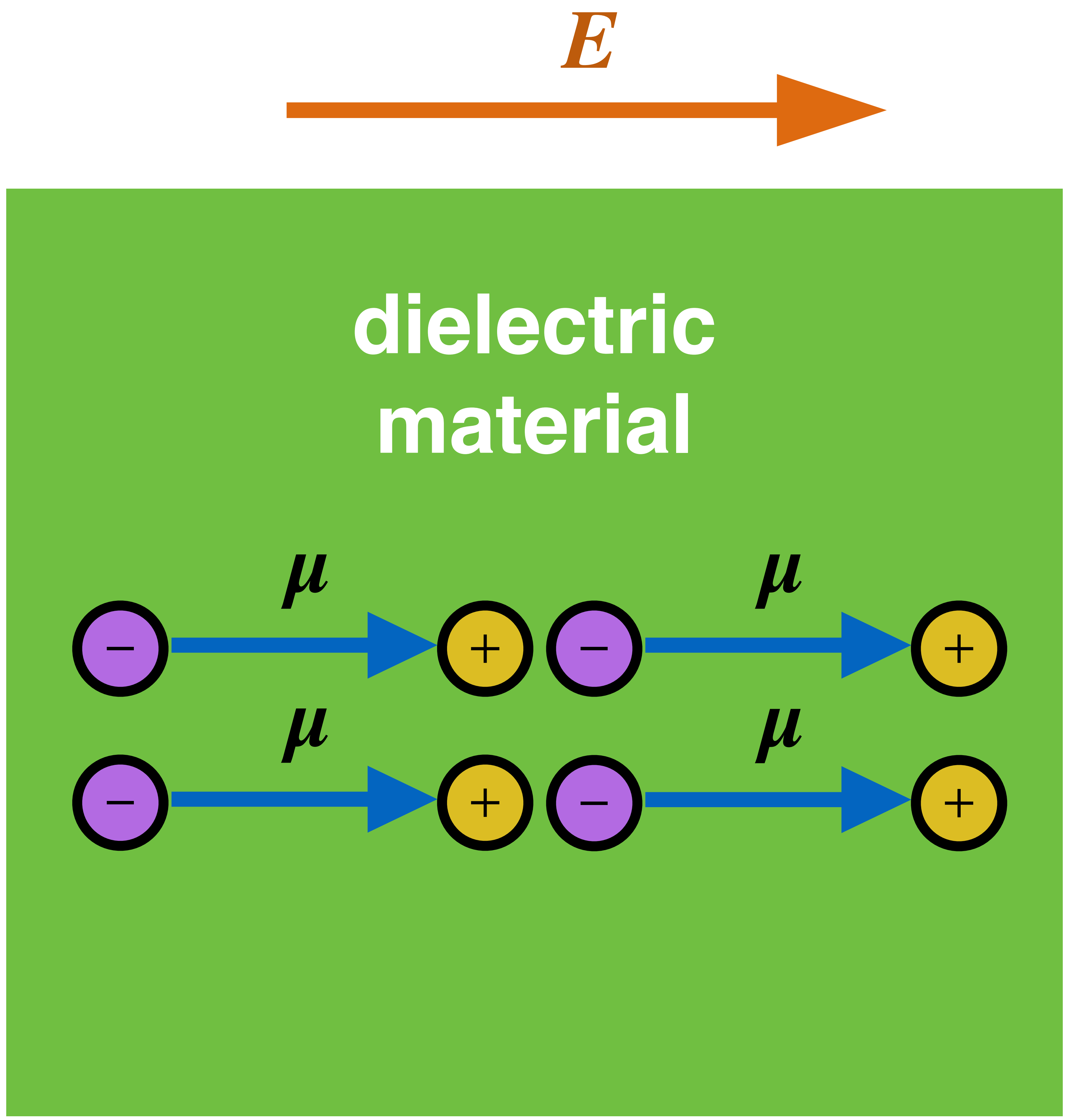
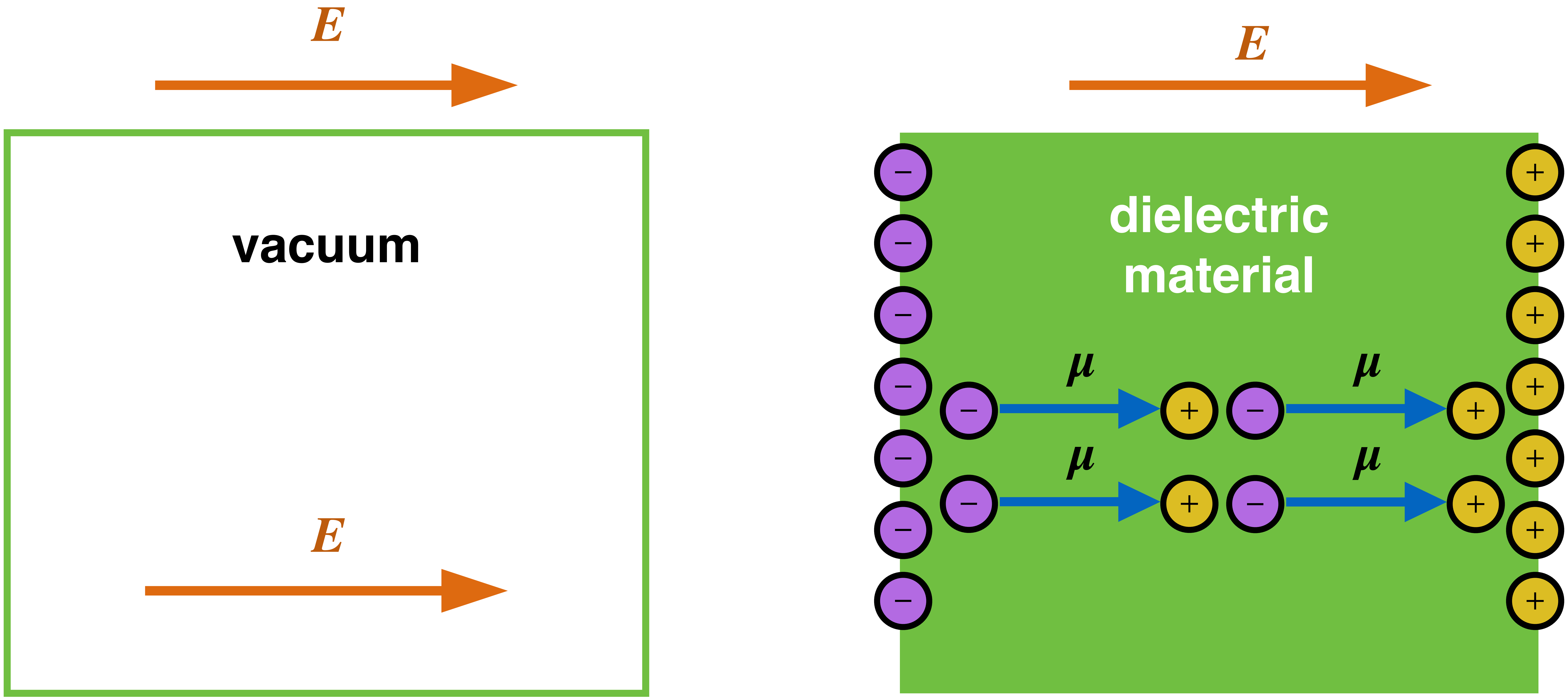




Dielectric materials

- Dielectric material: electrical insulator that can be polarised by applied electric field



Dielectric materials

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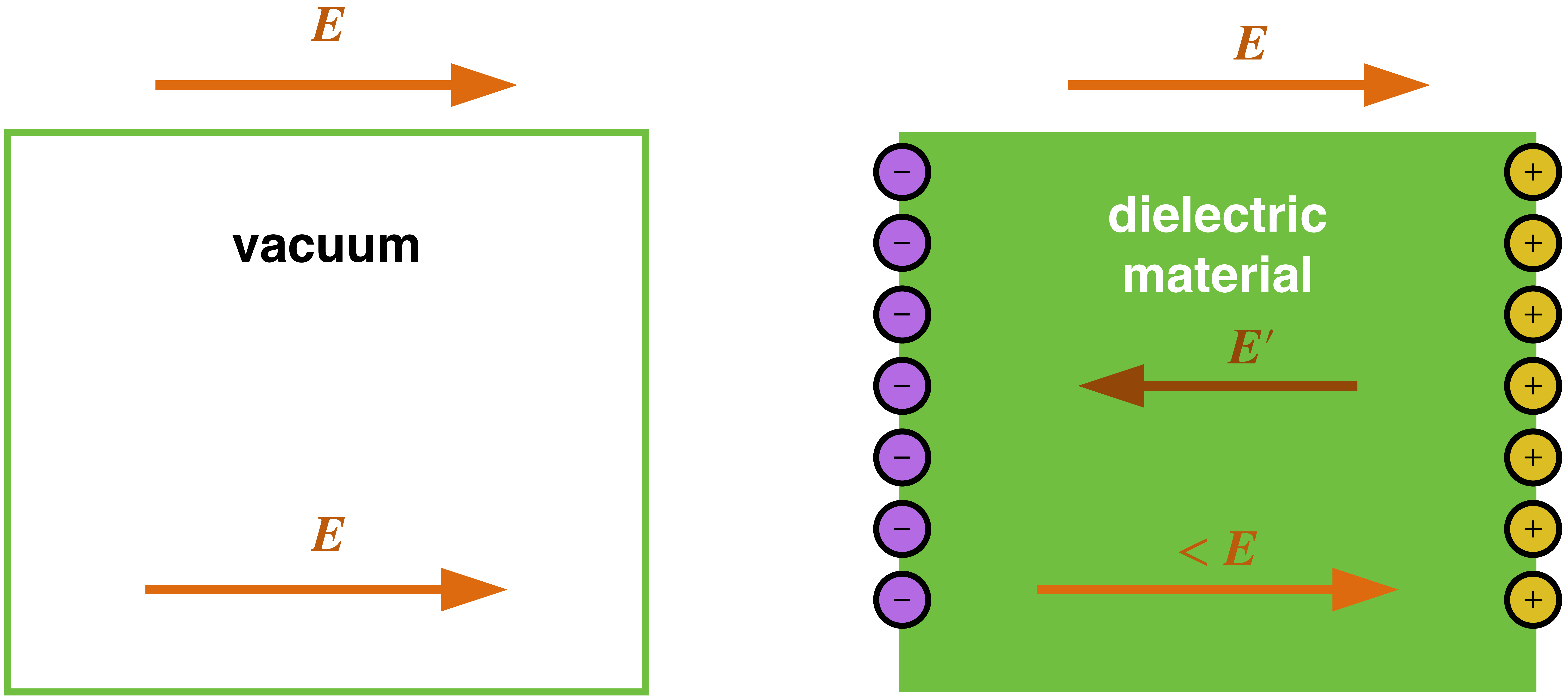
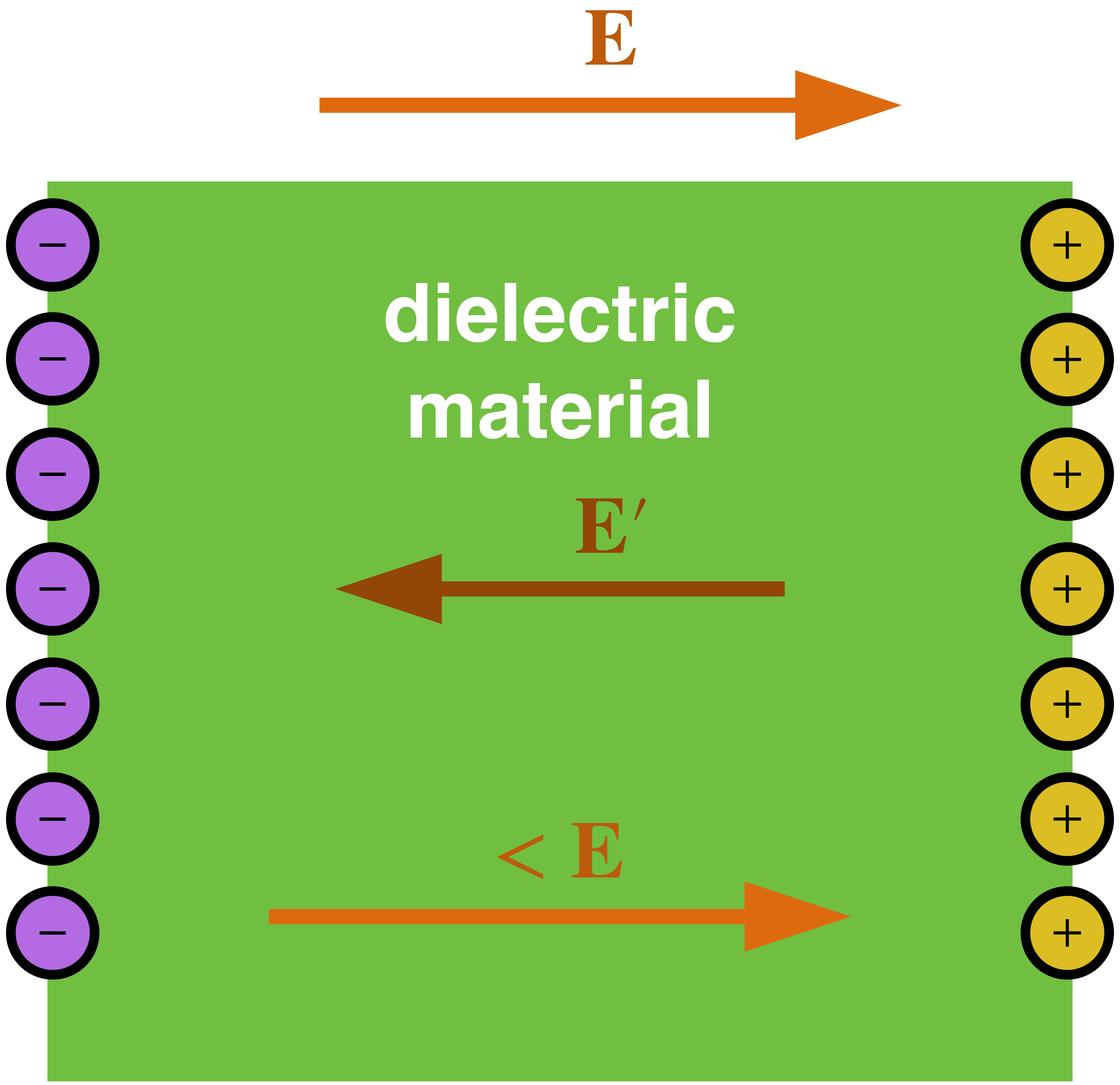


Dielectric materials



- Displacement field:

$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P}$$

$\boldsymbol{D}$: displacement field $[\mathrm{C m^{-2}}]$

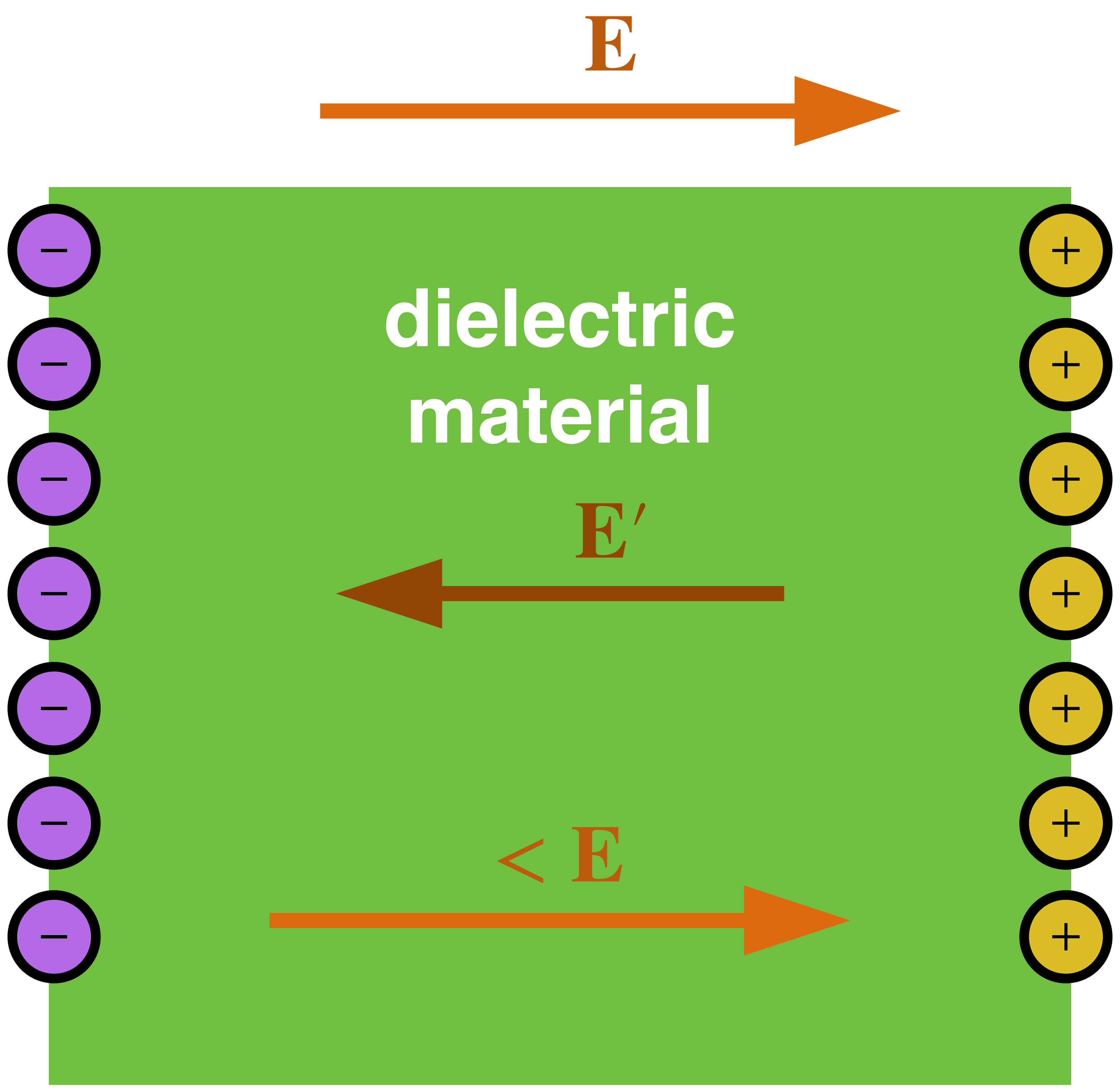
ε_0 : permittivity of free space $[8.85 \times 10^{-12}\,\mathrm{F m^{-1}}]$

$\boldsymbol{E}$: electric field $[\mathrm{V m^{-1}}]$

$\boldsymbol{P}$: polarisation $[\mathrm{C\,m^{-2}}]$

$$[\mathrm{F} = \mathrm{C\,V^{-1}}]$$

Dielectric materials



- Displacement field in linear, homogeneous, and isotropic dielectric with instantaneous response:

$$\boldsymbol{D} = \varepsilon \boldsymbol{E}$$

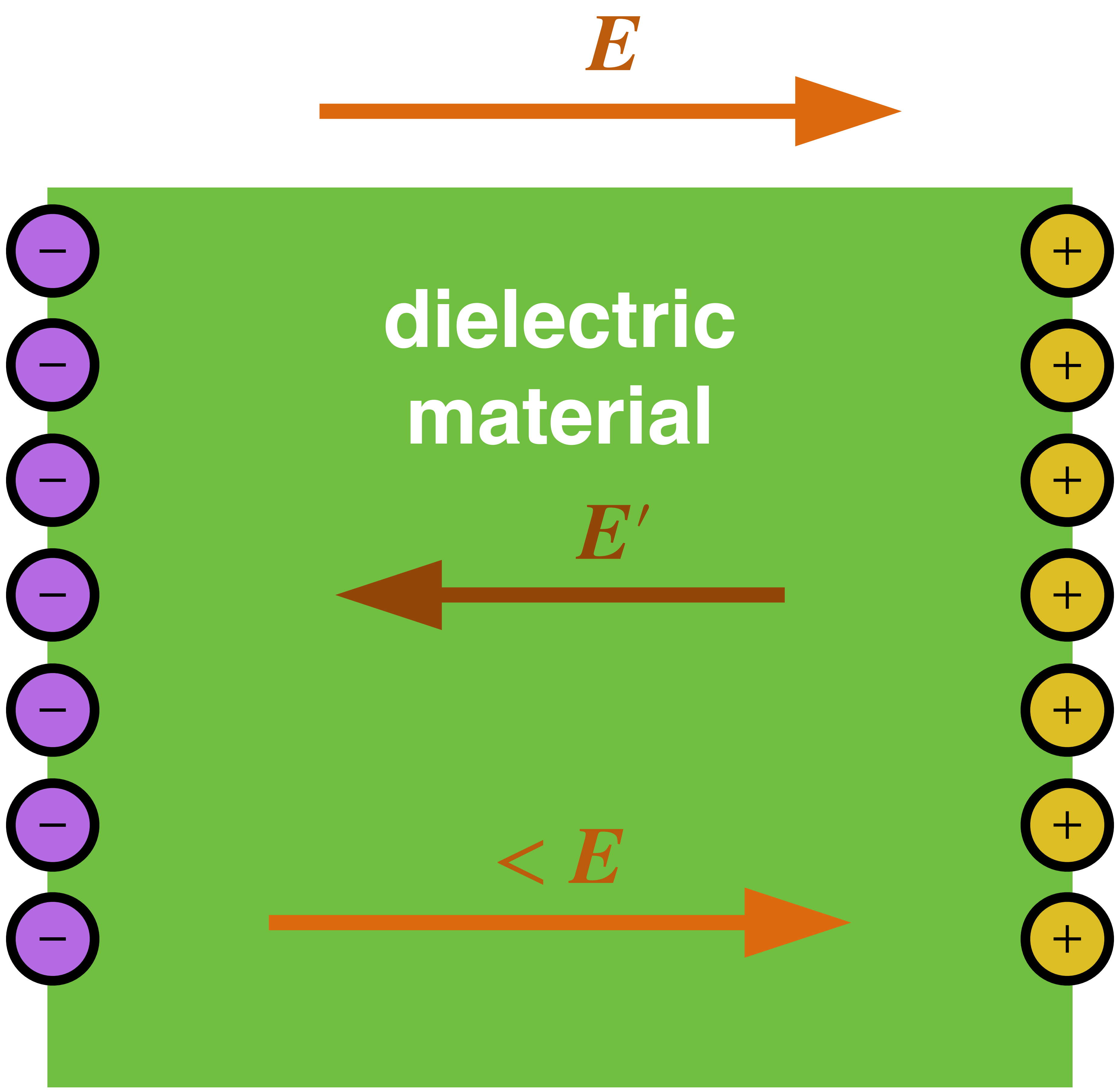
$\boldsymbol{E}$: electric field $[\mathrm{V m^{-1}}]$

$\boldsymbol{D}$: displacement field $[\mathrm{C m^{-2}}]$

ε : permittivity $[\mathrm{F m^{-1}}]$

$$[\mathrm{F = C\,V^{-1}}]$$

Dielectric materials



- Displacement field:

$$\boldsymbol{D} = \varepsilon \boldsymbol{E} = \kappa \varepsilon_0 \boldsymbol{E}$$

$\boldsymbol{E}$: electric field $[\mathrm{Vm^{-1}}]$

$\boldsymbol{D}$: displacement field $[\mathrm{Cm^{-2}}]$

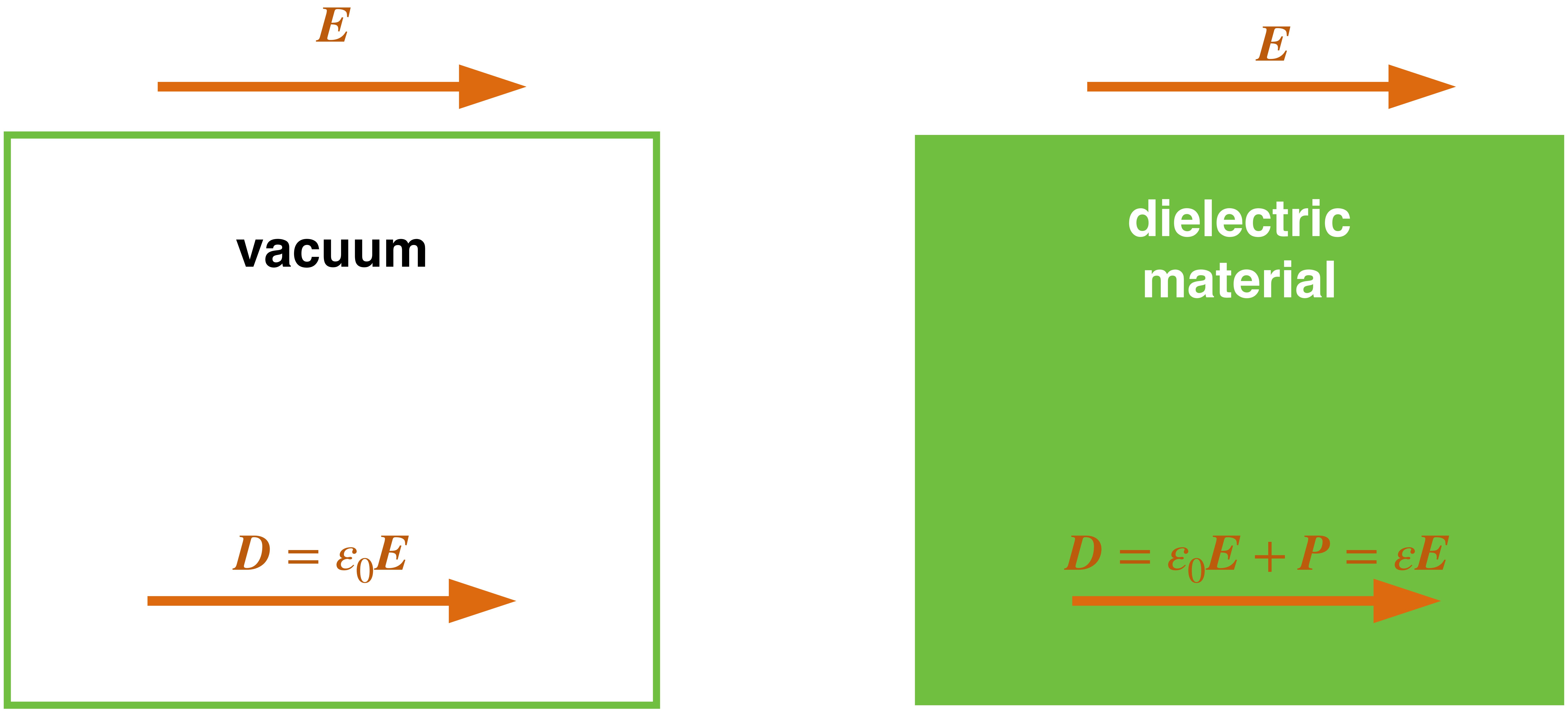
ε : permittivity $[\mathrm{Fm^{-1}}]$

ε_0 : permittivity of free space $[8.85 \times 10^{-12}\,\mathrm{Fm^{-1}}]$

$\kappa = \dfrac{\varepsilon}{\varepsilon_0}$: dielectric constant [dimensionless]

Dielectric materials

- Dielectric material: electrical insulator that can be polarised by applied electric field



Dielectric materials

- *See derivation of polarisation in terms of dielectric constant and susceptibility*

$$\boldsymbol{P} = \varepsilon_0 \boldsymbol{E}(\kappa - 1) = \varepsilon_0 \chi \boldsymbol{E}$$

Examples of dielectric materials

vacuum
(1)

air
(1.0006)

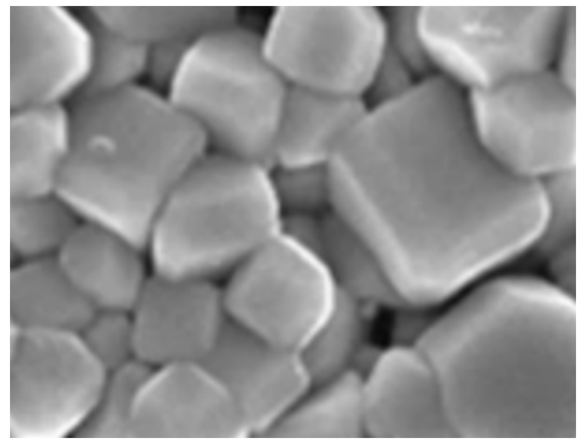
paper
(1.4)

glass
(3.7 – 10)

water
(50 – 90)

$BaTiO_3$
(1,200 – 10,000)

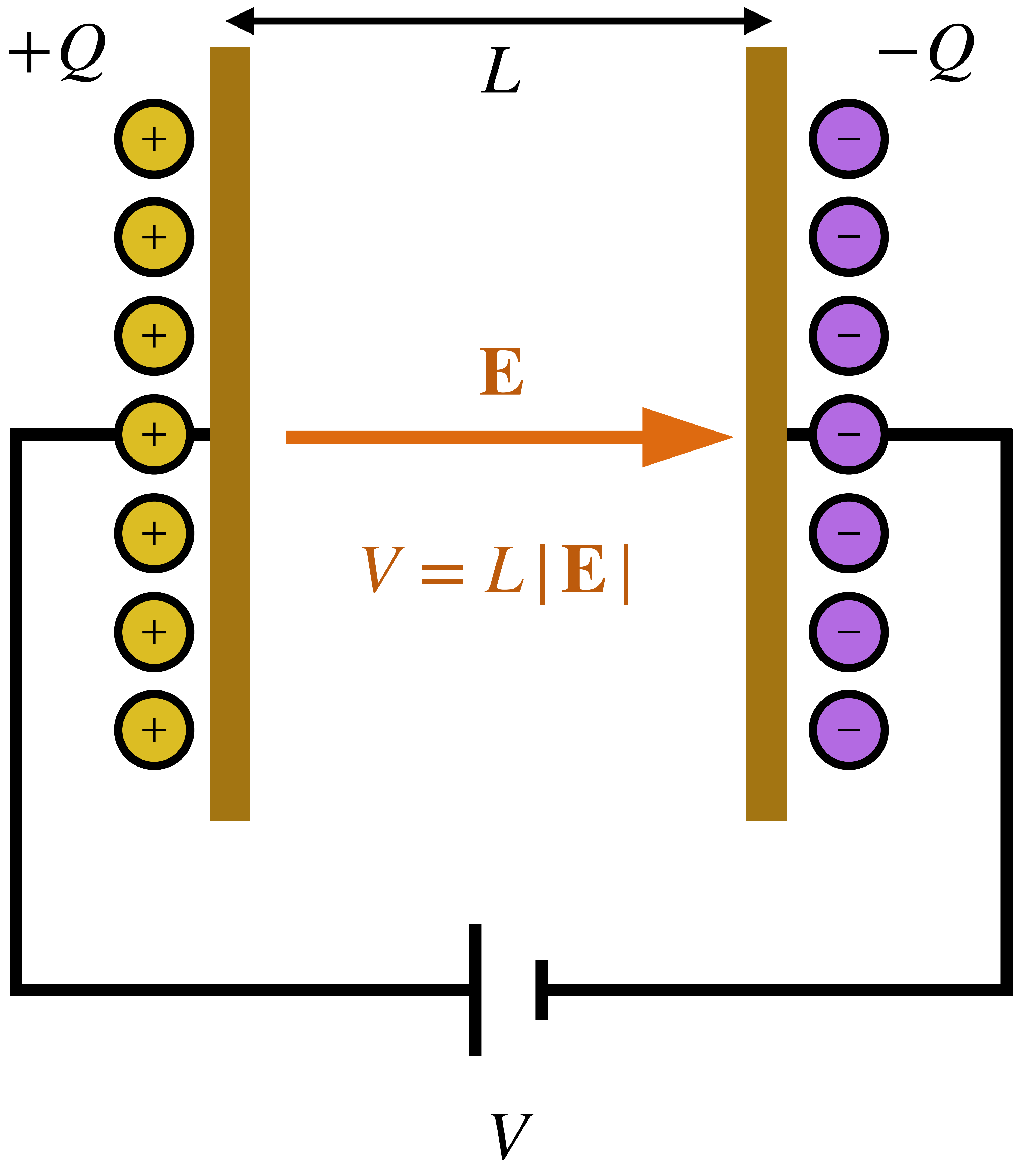
$CaCu_3Ti_4O_{12}$
(10,000 – 300,000)



1 — 10 — 100 — 1,000 — 10,000 — 100,000 → κ

Credit: Scherff [CC BY-SA 3.0] via Wikimedia Commons
José Manuel Suárez [CC BY-SA 2.0] via Wikimedia Commons
Materialscientist [CC BY-SA 3.0] via Wikimedia Commons
Scientific Reports 8, 1392 (2018)

Parallel plate capacitor



- Capacitance

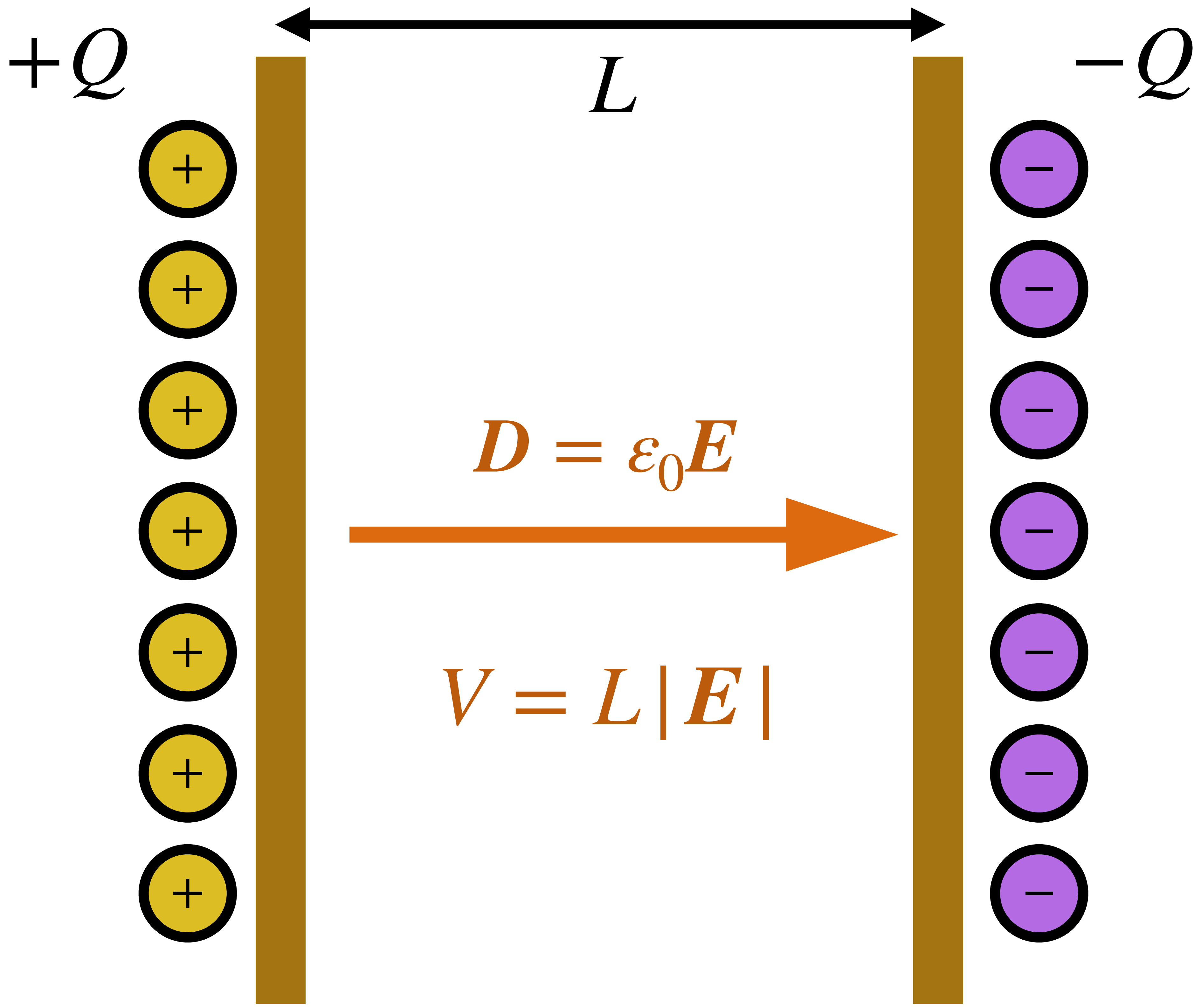
$$C = \frac{Q}{V} \quad [\mathrm{F} = \mathrm{C\,V^{-1}}]$$

Charge density on parallel plate capacitor

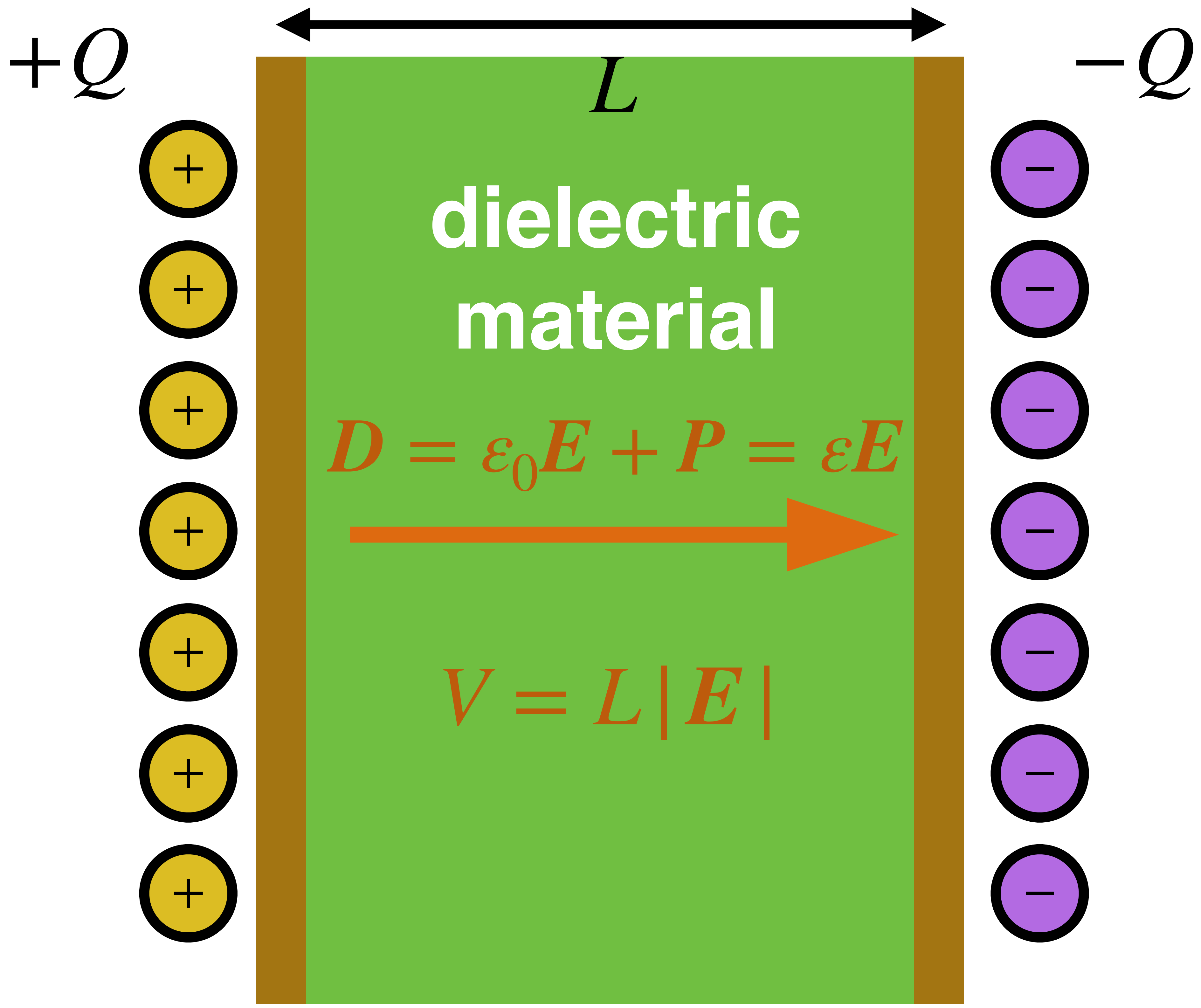
- *See derivation in handout Appendix A (non-examinable)*

$$\boxed{\sigma = \frac{Q_{\text{free}}}{A} = |\mathbf{D}|} \qquad [\mathrm{C\,m^{-2}}]$$

Parallel plate capacitor

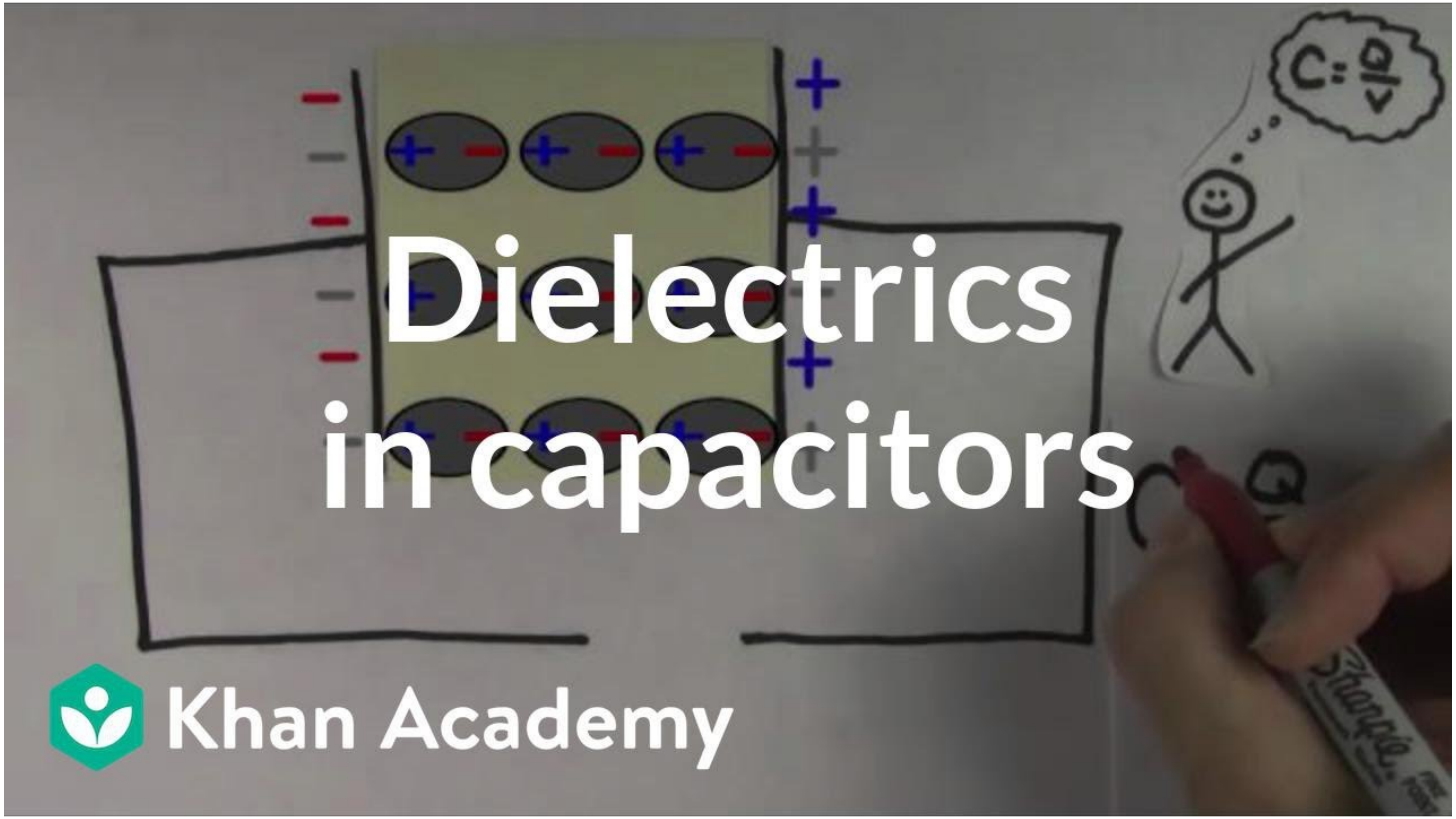


$$C = \frac{Q}{V} = \varepsilon_0 \frac{A}{L}$$



$$C = \frac{Q}{V} = \varepsilon \frac{A}{L}$$

Parallel plate capacitor: alternative explanation



Additional slides

Aside: Gauss's law

$$\boxed{\Phi_D = Q_{\text{free}}}$$

$$\Phi_D = \oint_S \mathbf{D} \cdot \mathrm{d}\mathbf{A}$$

Φ_D : displacement field flux over closed surface S [C]

Q_{free} : total free charge enclosed by surface S [C]

ε_0 : permittivity of free space [$8.85 \times 10^{-12}\,\mathrm{Fm}^{-1}$]

$\mathbf{D}$: displacement field [Cm^{-2}]

$\mathrm{d}\mathbf{A}$: infinitesimal area element of surface S [m^2]