# Dielectrics I [1119]

# Induced electric dipole moments:

Atoms in their ground state have zero electric dipole moment to very high precision. Atoms are polarizable by an electric field, which slightly displaces positive charge carriers (nuclei) and negative charge carriers (electrons) in opposite directions.

Induced electric dipole moment:  $\mathbf{p} \doteq q [\langle \mathbf{x}_+ \rangle - \langle \mathbf{x}_- \rangle] = \alpha \mathbf{E}.$ 

Atomic polarizability:  $\alpha$  [Cm<sup>2</sup>/V].

Practical scale:  $4\pi\epsilon_0 R^3$ , inferred from the dipole moment  $\mathbf{p} = 4\pi\epsilon_0 R^3 \mathbf{E}_{ap}$  of a conducting sphere in a uniform field  $\mathbf{E}_{ap}$ .

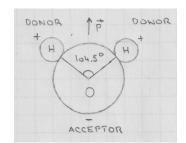
[lex17][lex217]

Empirical data for  $\alpha$  of selected elements compiled separately.

Calculation of  $\alpha$  via quantum mechanical perturbation theory.

# Result for hydrogen: $\frac{\alpha}{4\pi\epsilon_0 a_{\scriptscriptstyle \mathrm{B}}^3} = \frac{9}{2}.$

Bohr radius: 
$$a_{\rm B} = \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \simeq 5.29 \times 10^{-11} {\rm m}.$$



# Polar molecules:

[lam16]

Some molecules have a permanent electric dipole moment.

Practical unit:  $1D = 3.34 \times 10^{-30}$ Cm (Debye).

Dipole moment of H<sub>2</sub>O molecule: p = 1.8546D.

Comparative scale:  $ea_{\rm B} \simeq 2.5 \,\mathrm{D}$ .

Polar molecules in gases or liquids have random orientation. Due to thermal fluctuations, the average dipole moment of a polar molecule is zero:  $\langle \mathbf{p} \rangle = 0$ .

An external electric field  $\mathbf{E} = E_0 \hat{\mathbf{k}}$  exerts a torque  $\mathbf{p} \times \mathbf{E}$  on polar molecules, which tends to align the dipole moments parallel to the field.

The average dipole moment is then the result of a statistical mechanical problem. The resulting mathematical expression is better known in a different physical context (Langevin paramagnet):

$$\langle \mathbf{p} \rangle \cdot \hat{\mathbf{k}} = p \left[ \coth x - \frac{1}{x} \right], \quad x \doteq \frac{pE_0}{k_{\rm B}T}.$$

$$\langle \mathbf{p} \rangle \xrightarrow{pE_0 \ll k_{\rm B}T} \alpha \mathbf{E}, \quad \alpha = \frac{p^2}{3k_{\rm B}T}.$$

# Polarization and bound charge:

We introduce a vector-field quantity representing the average dipole-moment density at the center of a mesoscopic region of space.

$$\Rightarrow \Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int_V d^3 x' \left[ \nabla' \cdot \left( \frac{\mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \right) - \frac{\nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \right].$$

[gmd1-B]

 $\triangleright$  Use Gauss's theorem for first term:

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \oint_S da' \frac{\hat{\mathbf{n}} \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} - \frac{1}{4\pi\epsilon_0} \int_V d^3x' \frac{\nabla' \cdot \mathbf{P}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}$$

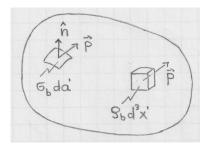
 $\triangleright$  Identify bound surface and volume charge densities in integrals:

[lex29]

$$\sigma_{\rm b} = \hat{\mathbf{n}} \cdot \mathbf{P} \quad [\mathrm{C/m^2}], \quad \rho_{\rm b} = -\nabla \cdot \mathbf{P} \quad [\mathrm{C/m^3}].$$
  
$$\Rightarrow \quad \Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \oint_S da' \frac{\sigma_{\rm b}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} + \frac{1}{4\pi\epsilon_0} \int_V d^3x' \frac{\rho_{\rm b}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|}.$$

Uniform polarization produces bound surface charge density, but no volume charge density.

Bound charge, like free charge, is the source of an electric field.



#### **Displacement field:**

Fundamental equations of electrostatics:  $\nabla \times \mathbf{E} = 0$ ,  $\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$ . Density of free and bound charge on dielectric:  $\rho(\mathbf{x}) = \rho_f(\mathbf{x}) + \rho_b(\mathbf{x})$ . Free charge is excess charge. It is not, in general, mobile charge. Polarization charge density:  $\rho_b(\mathbf{x}) = -\nabla \cdot \mathbf{P}(\mathbf{x})$ .

Gauss's law for electric field:

 $\triangleright \text{ integral version: } \epsilon_0 \oint_S \mathbf{E} \cdot d\mathbf{a} = Q^{(\text{in})},$  $\triangleright \text{ differential version: } \epsilon_0 \nabla \cdot \mathbf{E} = \rho,$  $\triangleright \text{ application to dielectric: } \epsilon_0 \nabla \cdot \mathbf{E} = \rho_{\text{f}} + \rho_{\text{b}} = \rho_{\text{f}} - \nabla \cdot \mathbf{P}.$ 

Consequence:  $\rho_{\rm f} = \nabla \cdot [\epsilon_0 \mathbf{E} + \mathbf{P}].$ 

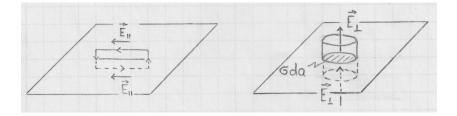
Displacement field:  $\mathbf{D}(\mathbf{x}) \doteq \epsilon_0 \mathbf{E}(\mathbf{x}) + \mathbf{P}(\mathbf{x}) \quad [C/m^2].$ 

Gauss's law for displacement field:

▷ differential version:  $\nabla \cdot \mathbf{D} = \rho_{\rm f}$ , ▷ integral version:  $\oint_{S} \mathbf{D} \cdot d\mathbf{a} = Q_{\rm f}^{\rm (in)}$ .

## Boundary conditions involving dielectrics:

- $\triangleright$  Electric field **E** at dielectric interface or surface:
  - Electrostatic field is irrotational:  $\nabla \times \mathbf{E} = 0$ .
  - Consequence: The tangential part of the electric field is continuous at the surface/interface:  $\Delta \mathbf{E}_{\parallel} = 0$ .
  - Presence of bound and/or free surface charge:  $\sigma = \sigma_{\rm b} + \sigma_{\rm f}$ .
  - Consequence: The normal part of the electric is discontinuous at the surface/interface:  $\Delta \mathbf{E}_{\perp} = \sigma/\epsilon_0$ .



- $\triangleright$  Displacement field **D** at dielectric interface or surface:
  - Gauss's law for the displacement field reads,  $\nabla \cdot \mathbf{D} = \rho_{\rm f}$ .
  - Consequence: The normal component of the displacement field is continuous at a surface/interface with only bound charge  $\sigma_{\rm b}$ present:  $\Delta \mathbf{D}_{\perp} = 0$ . It is discontinuous if also free charge  $\sigma_{\rm f}$  is present at the surface/interface:  $\Delta \mathbf{D}_{\perp} = \sigma_{\rm f}$ .
  - The displacement field **D** is not, in general, irrotational.
  - Consequence: The tangential part  $\mathbf{D}_{\parallel}$  of the displacement is not necessarily continuous at the surface/interface.

#### Linear dielectrics:

The relation between the fields  $\mathbf{E}$  and  $\mathbf{D}$  requires a *constitutive equation* based on empirical data.

Gases, liquids, and amorphous solids are *isotropic* dielectrics. Crystalline matter is, in general, an *anisotropic* dielectric.

In electric fields that are not too strong, the relation between the fields  $\mathbf{E}$  and  $\mathbf{D}$  is *linear*.

In linear dielectrics, the strength (magnitude) of **E** and **D** are proportional to one another. In isotropic dielectrics, the directions of **E** and **D** are the same, whereas in anisotropic dielectrics, the directions are, in general, different.

Linear dielectric crystalline matter is described by tensor relations (a more advanced topic).

Isotropic linear dielectrics are specified by one of three alternative material parameters:

- susceptibility:  $\chi_{\rm e}$ ,
- permittivity:  $\epsilon$ ,
- dielectric constant:  $\kappa$ .

Linear relations:  $\mathbf{P} = \chi_{e} \epsilon_0 \mathbf{E}, \quad \mathbf{D} = \epsilon \mathbf{E} = \kappa \epsilon_0 \mathbf{E}.$ 

Relations between material parameters:  $\epsilon = \kappa \epsilon_0 = (1 + \chi_e)\epsilon_0$ .

[lam16] Tabulated data of dielectric constant are compiled separately.

[lex30][lex32] [lex48][lex199] [lex200]

#### Poisson equation for uniform linear dielectric:

Linear dielectric:  $\mathbf{D} = \epsilon \mathbf{E} = -\epsilon \nabla \Phi$ .

Uniform linear dielectric:  $\epsilon = \text{const.}$ 

Gauss's laws for **E** and **D**:  $\epsilon_0 \nabla \cdot \mathbf{E} = \rho_f + \rho_b$ ,  $\nabla \cdot \mathbf{D} = \rho_f$ .

Two versions of the Poisson equation follow:

$$\Rightarrow -\nabla^2 \Phi = \frac{\rho_{\rm f}}{\epsilon}, \quad -\nabla^2 \Phi = \frac{\rho_{\rm f} + \rho_{\rm b}}{\epsilon_0}.$$

Consistency implies the following relation between the densities of bound and free charge in a uniform linear dielectric:

$$\Rightarrow \rho_{\rm b}(\mathbf{x}) = \left(\frac{1}{\kappa} - 1\right) \rho_{\rm f}(\mathbf{x}) \quad \text{or} \quad \epsilon \rho_{\rm b}(\mathbf{x}) = (\epsilon_0 - \epsilon) \rho_{\rm f}(\mathbf{x}).$$

Note that bound-charge and free-charge densities at any given location have opposite sign.

#### Clausius-Mossotti model:

Thus far we have described effects electric polarization on the microscopic level by introducing the polarizability  $\alpha$  and on the macroscopic level by introducing the dielectric constant  $\kappa$ .

The relation between the two descriptions (one discrete, the other continuous) is far from straightforward.

The Clausius-Mossotti model takes into account that the electric field which is responsible for the polarization of an atom must exclude the electric field that is the result of its own polarization:

$$\mathbf{p} = \alpha (\mathbf{E} - \mathbf{E}_{\mathrm{s}}).$$

What the field  $\mathbf{E}_{s}$  is, is not easy to establish. The Clausius-Mossotti model uses the field inside a uniformly polarized sphere for that purpose: [lex29]

$$\mathbf{E}_{s} = -\frac{\mathbf{P}}{3\epsilon_{0}} = -\frac{n\mathbf{p}}{3\epsilon_{0}}; \quad n = \frac{1}{v}, \quad v = \frac{4\pi}{3}a^{3}.$$

The bridge between  $\alpha$  and  $\kappa$  can thus be built as follows:

$$\mathbf{P} = n\alpha \left( \mathbf{E} + \frac{\mathbf{P}}{3\epsilon_0} \right) = \chi_e \epsilon_0 \mathbf{E} \quad \Rightarrow \quad \chi_e = \frac{3n\alpha}{3\epsilon_0 - n\alpha} \quad \Rightarrow \quad \alpha = \frac{3\epsilon_0}{n} \frac{\kappa - 1}{\kappa + 2}.$$

#### Energy density in dielectric:

Derivation for a situation with bulk free-charge density  $\rho_{\rm f}(\mathbf{x})$ , which determines the bulk bound-charge density  $\rho_{\rm b}(\mathbf{x})$  as discussed earlier.

Augmentation of free charge within dielectric:  $\delta \rho_{\rm f}(\mathbf{x})$ .

Increment of electrostatic potential energy:  $\delta U = \int d^3x \delta \rho_{\rm f}(\mathbf{x}) \Phi(\mathbf{x}).$ 

Gauss's law for displacement field:  $\delta \rho_{\rm f}(\mathbf{x}) = \nabla \cdot \delta \mathbf{D}(\mathbf{x}).$ 

Integration by parts:  $\int d^3x \, [\nabla \cdot \delta \, \mathbf{D}(\mathbf{x})] \Phi(\mathbf{x}) = \int d^3x \, \delta \, \mathbf{D}(\mathbf{x}) \cdot [-\nabla \Phi(\mathbf{x})].$ Transformation of integrand:

$$\delta \mathbf{D} \cdot [-\nabla \Phi] = \delta \mathbf{D} \cdot \mathbf{E} = \epsilon \delta \mathbf{E} \cdot \mathbf{E} = \frac{1}{2} \epsilon \delta (\mathbf{E} \cdot \mathbf{E}) = \frac{1}{2} \delta (\mathbf{D} \cdot \mathbf{E}).$$
  
$$\Rightarrow \ \delta U = \int d^3 x \, \frac{1}{2} \delta (\mathbf{D}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x})) = \delta \left(\frac{1}{2} \int d^3 x \, \mathbf{D}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x})\right).$$

Electrostatic energy stored in dielectric:

$$U = \frac{1}{2} \int d^3 x \, \mathbf{D}(\mathbf{x}) \cdot \mathbf{E}(\mathbf{x}).$$

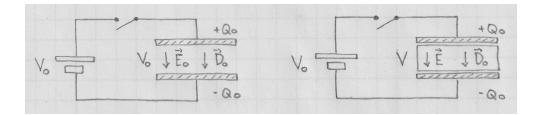
#### Capacitance with dielectric:

Parallel-plate geometry: area A, width d. Free charge on plates:  $Q = \sigma_{\rm f} A$ . Displacement field:  $D = \sigma_{\rm f}$  (inferred from Gauss's law). Electric field:  $E = D/\epsilon$ . Polarization:  $P = \chi_{e} \epsilon_0 E = \sigma_{b}$ . Charge densities:  $\frac{\sigma_{\rm b}}{\sigma_{\rm f}} = \frac{P}{D} = \frac{\chi_{\rm e}\epsilon_0 E}{\epsilon E} = \frac{\kappa - 1}{\kappa}.$ Voltage:  $\Delta \Phi \doteq V = Ed = \frac{Qd}{\epsilon A}.$ Capacitance:  $C \doteq \frac{Q}{V} = \frac{\epsilon A}{d} = \kappa C_{\text{vac}}.$ Dielectrics enhance capacitance.

[lex44][lex45]

## Impact of dielectric added to capacitor:

Case #1: Two identical capacitors are charged up without dielectric and then disconnected from the voltage source. Then a dielectric is inserted into one of the capacitors.



|                    | vacuum                            | dielectric   |
|--------------------|-----------------------------------|--|
|                    |                                   |  |
| charge             | $Q_0$                             | $Q = Q_0$ $D = D_0$  |
| displacement field | $D_0$                             | $D = D_0$  |
| electric field     | $E_0 = \frac{D_0}{\epsilon_0}$    | $E = \frac{D}{\epsilon} = \frac{E_0}{\kappa} < E_0$          |
| voltage            | $V_0$                             | $V = \frac{V_0}{\kappa} < V_0$                               |
| capacitance        | $C_0 = \frac{Q_0}{V_0}$           | $C = \frac{Q}{V} = \kappa C_0 > C_0$                         |
| potential energy   | $U_0 = \frac{Q_0^2}{2C_0}$        | $U = \frac{Q^2}{2C} = \frac{U_0}{\kappa} < U_0$              |
| energy density     | $u_E^{(0)} = \frac{1}{2} D_0 E_0$ | $u_E = \frac{1}{2}DE = \frac{u_E^{(0)}}{\kappa} < u_E^{(0)}$ |

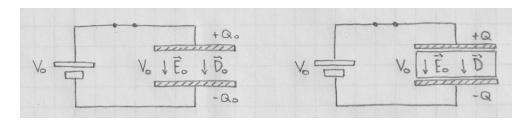
Inserting the dielectric leaves the charge on the plates invariant, but lowers the voltage across them.

The electric field decreases with the voltage when the dielectric is added, but the displacement field remains the same.

The energy density goes down because the electric field decreases. Where does that energy go? The answer is worked out in the exercises. [lex31]

The capacitance is a device property. It always increases when a dielectric is inserted, no matter what the circumstances are.

Case #2: Two identical capacitors without dielectric are charged up and then remain connected with the voltage source. Then a dielectric is inserted into one of the capacitors.



|                    | vacuum                            | dielectric   |
|--------------------|-----------------------------------|--|
|                    |                                   |  |
| voltage            | $V_0$                             | $V = V_0$ $E = E_0$                                  |
| electric field     | $E_0$                             | $E = E_0$  |
| displacement field | $D_0 = \epsilon_0 E_0$            | $D = \epsilon E = \kappa D_0 > D_0$                  |
| charge             | $Q_0$                             | $Q = \kappa Q_0 > Q_0$                               |
| capacitance        | $C_0 = \frac{Q_0}{V_0}$           | $C = \frac{Q}{V} = \kappa C_0 > C_0$                 |
| potential energy   | $U_0 = \frac{1}{2}C_0 V_0^2$      | $U = \frac{1}{2}CV^2 = \kappa U_0 > U_0$             |
| energy density     | $u_E^{(0)} = \frac{1}{2} D_0 E_0$ | $u_E = \frac{1}{2}DE = \kappa u_E^{(0)} > u_E^{(0)}$ |

Inserting the dielectric leaves the voltage across the plates invariant, but augments the charge on them.

The electric field remains constant with the voltage when the dielectric is added, but the displacement field now increases.

The energy density goes up because the displacement field increases. Where does that energy come from? The answer is worked out in the exercises.

[lex31]

The capacitance is a device property. It always increases when a dielectric is inserted, no matter what the circumstances are.

It is instructive to compare the insertion of dielectric materials and the insertion of conducting materials (without contact) between capacitor plates.

[lex53][lex54]