

Electric polarisation in materials

Lecture 2

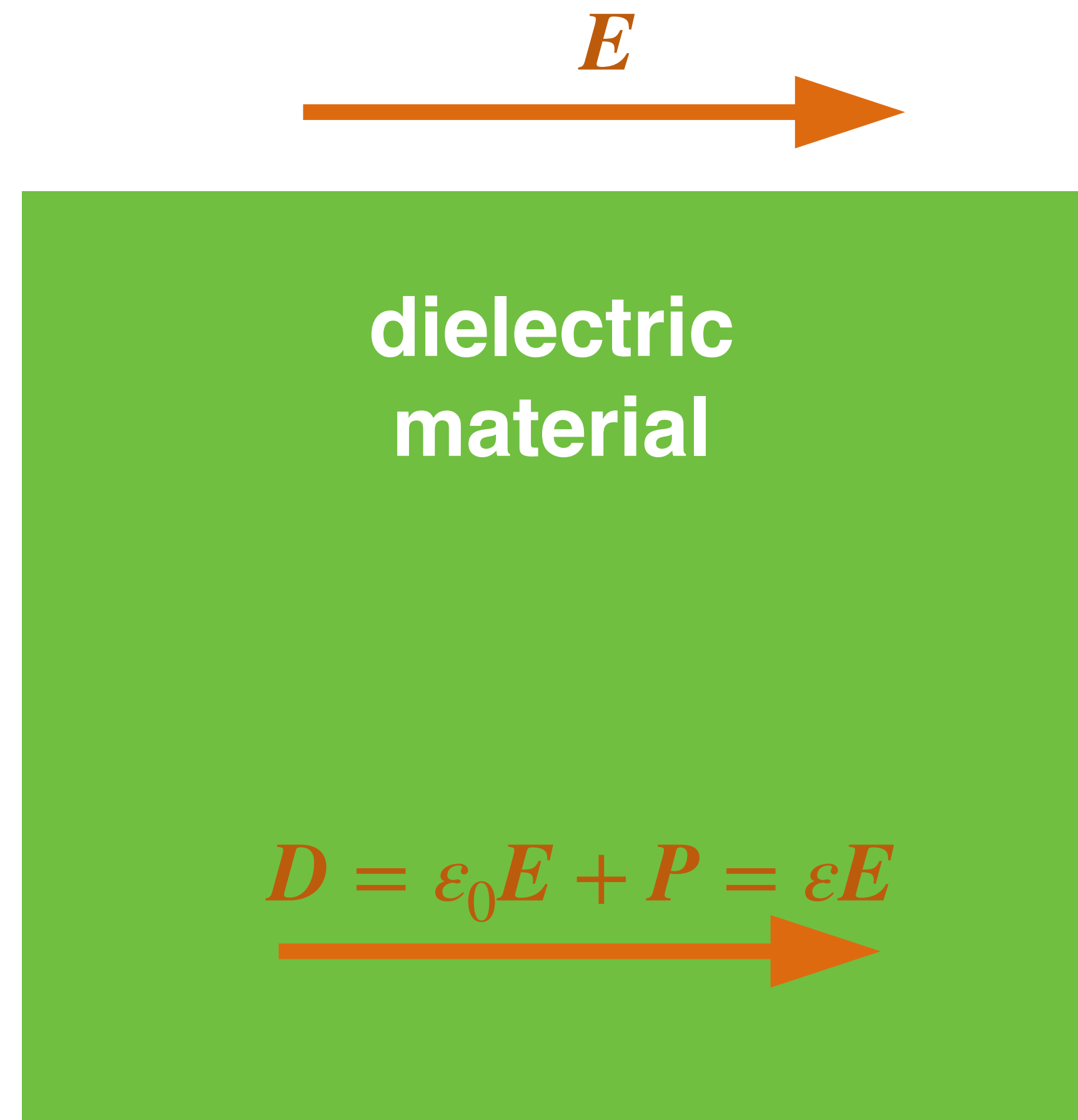
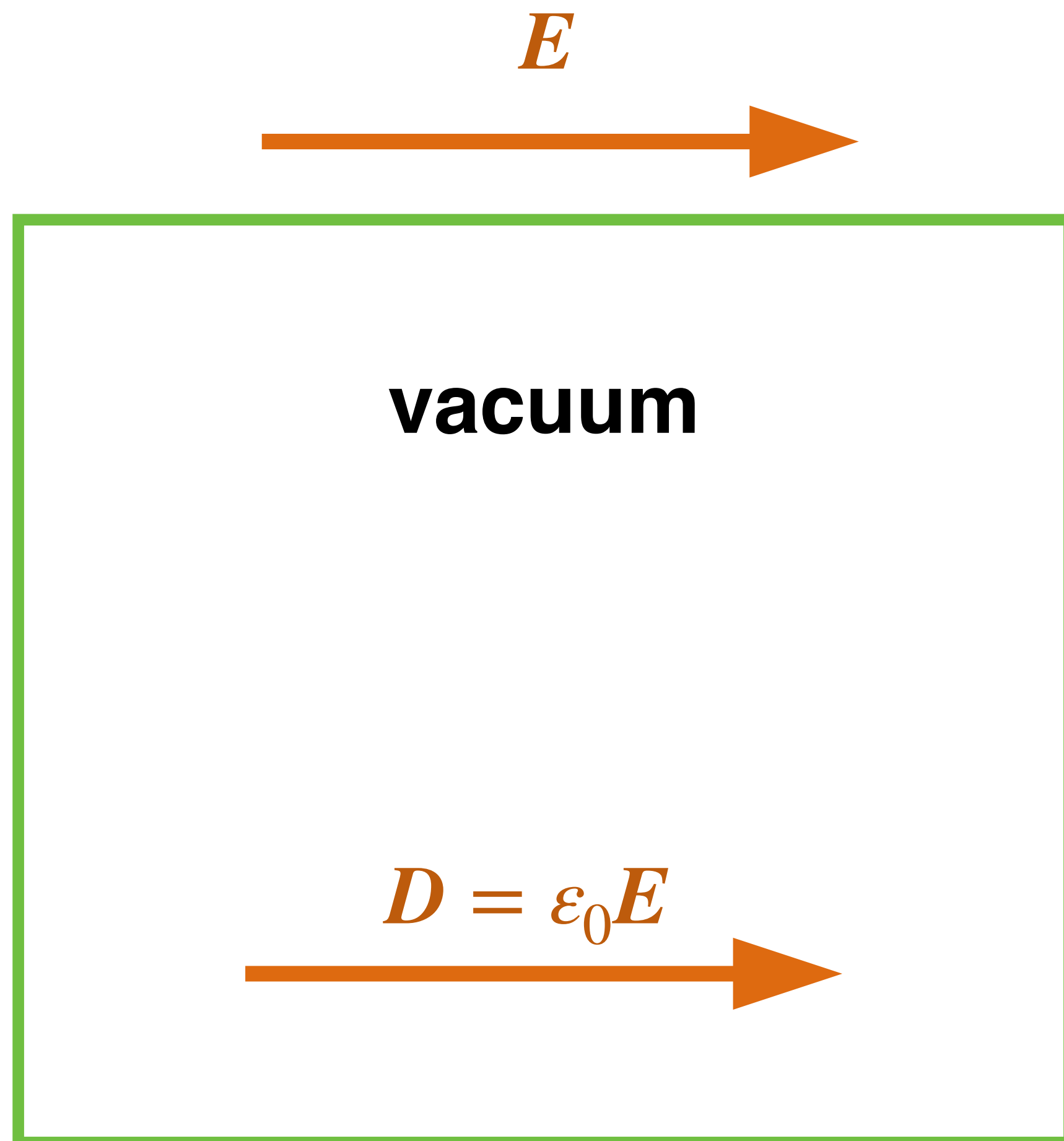
Bartomeu Monserrat
Course B: Materials for Devices

 Professor M does Science

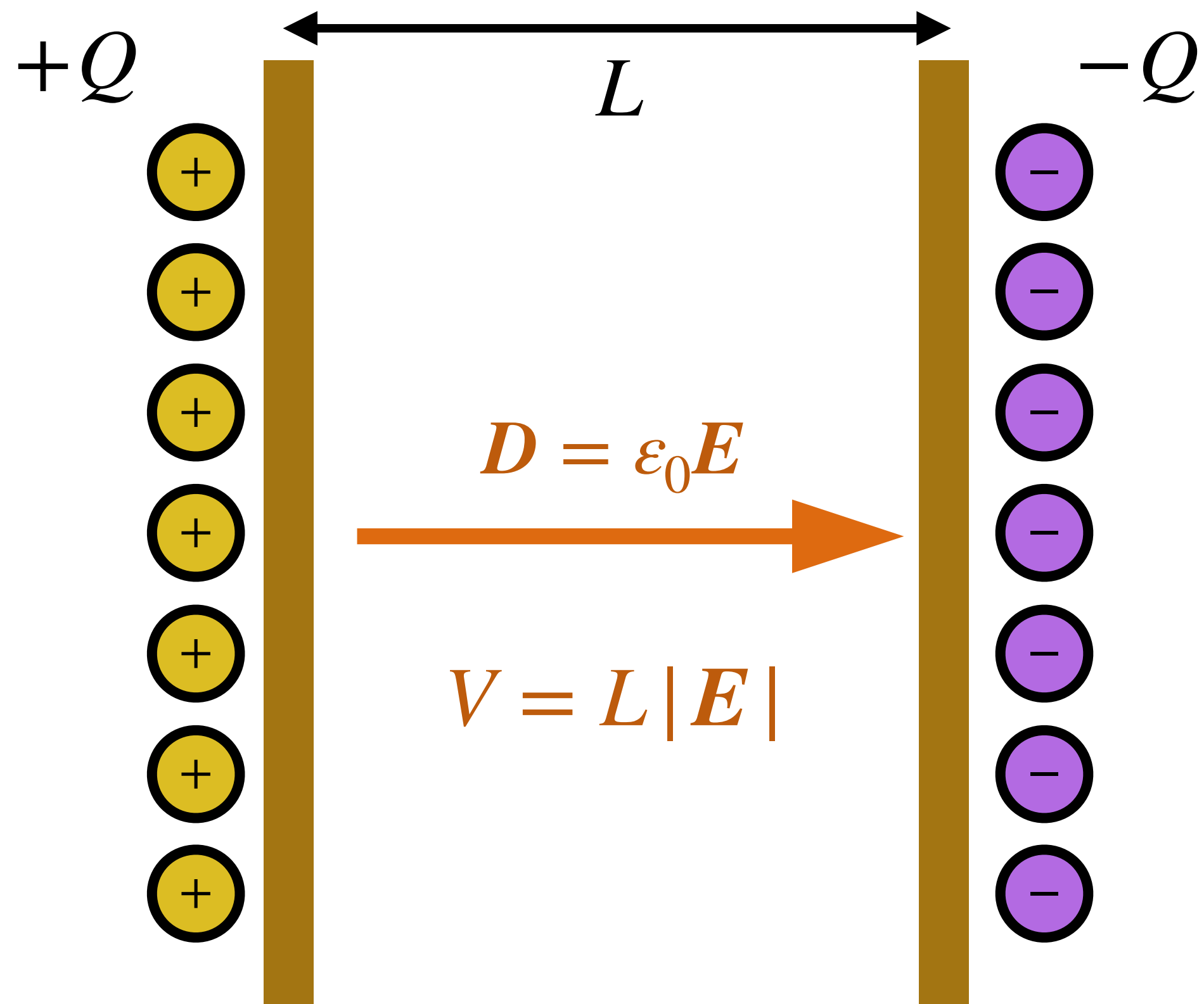
 <http://www.tcm.phy.cam.ac.uk/~bm418/>

Dielectric materials

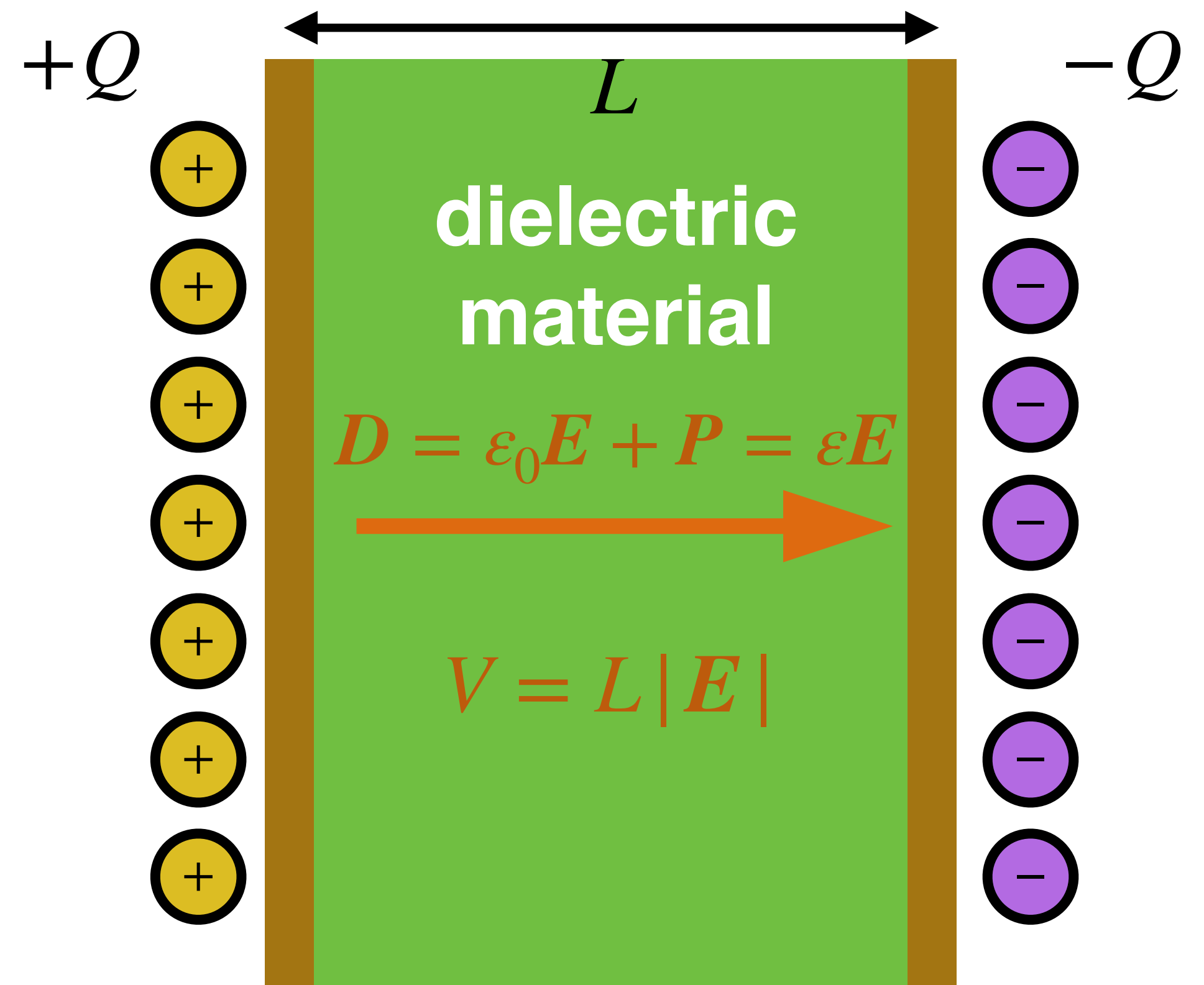
- Dielectric material: electrical insulator that can be polarised by applied electric field



Parallel plate capacitor



$$C = \frac{Q}{V} = \epsilon_0 \frac{A}{L}$$

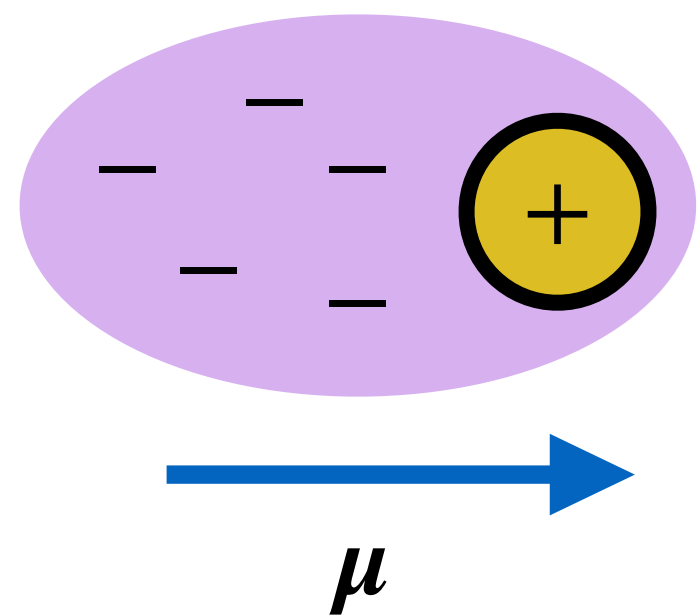
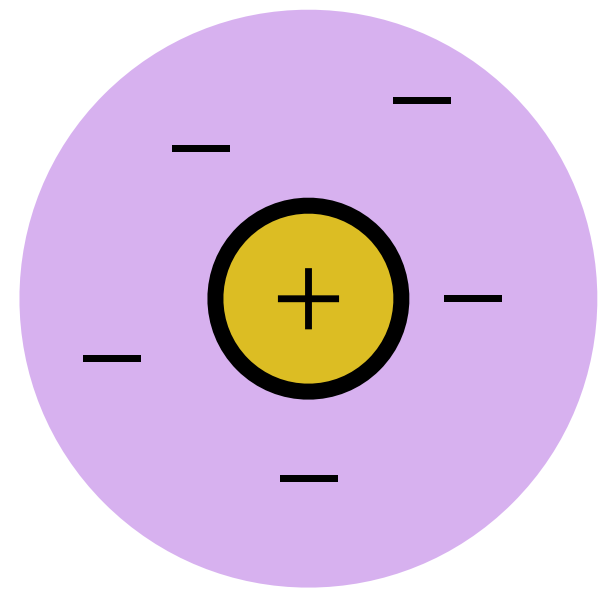


$$C = \frac{Q}{V} = \epsilon \frac{A}{L}$$

Polarisation mechanisms

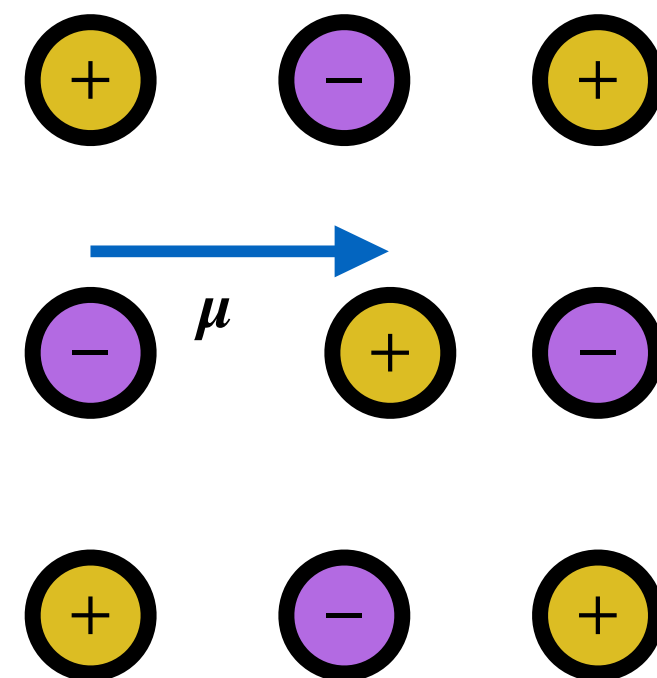
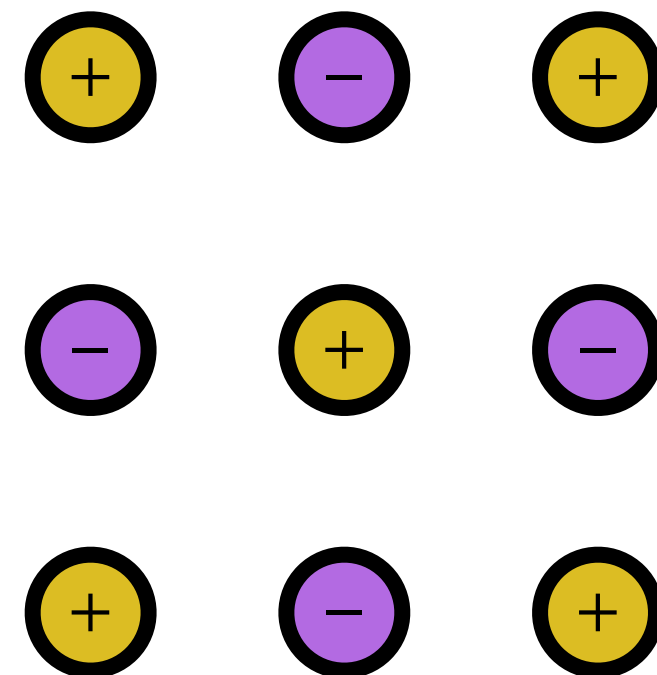
electronic
polarisation

$$\mathbf{E} = 0$$



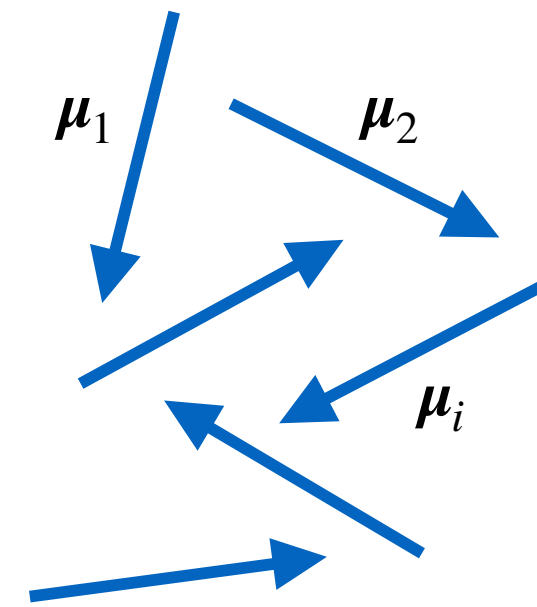
ionic
polarisation

$$\mu = 0$$

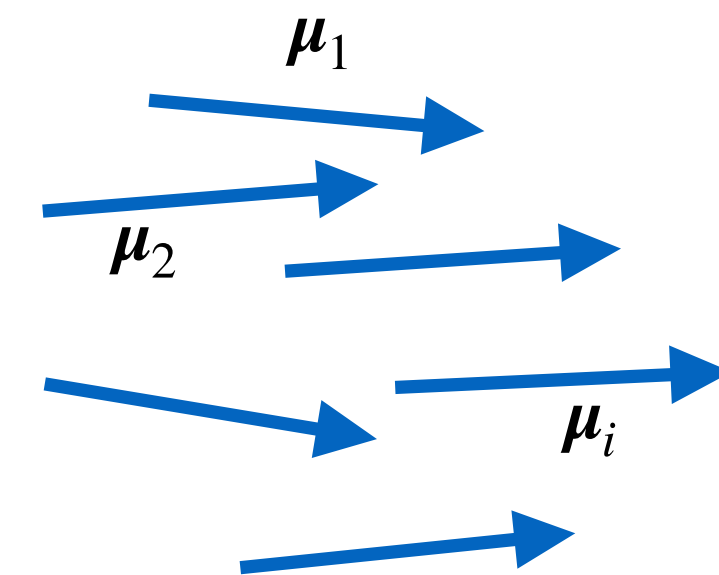


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orientation
polarisation



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

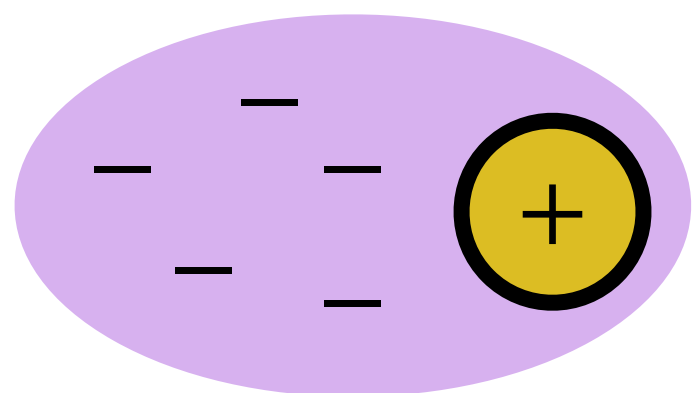
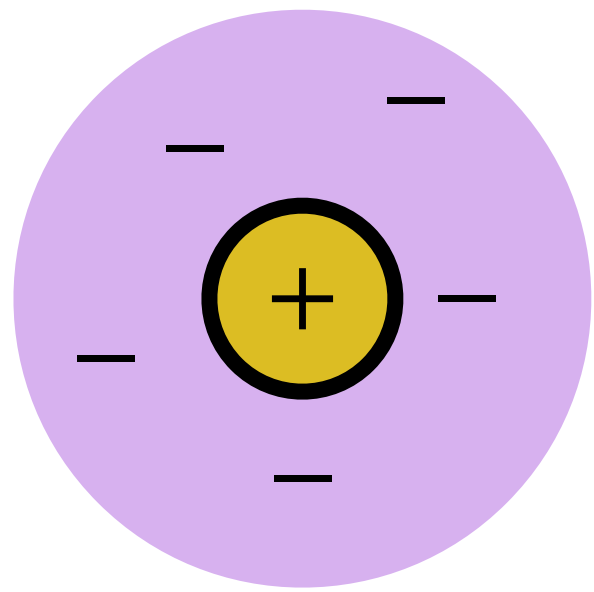


$$\mu = \sum_{i=1}^N \mu_i \simeq N\mu_1$$

Polarisation mechanisms

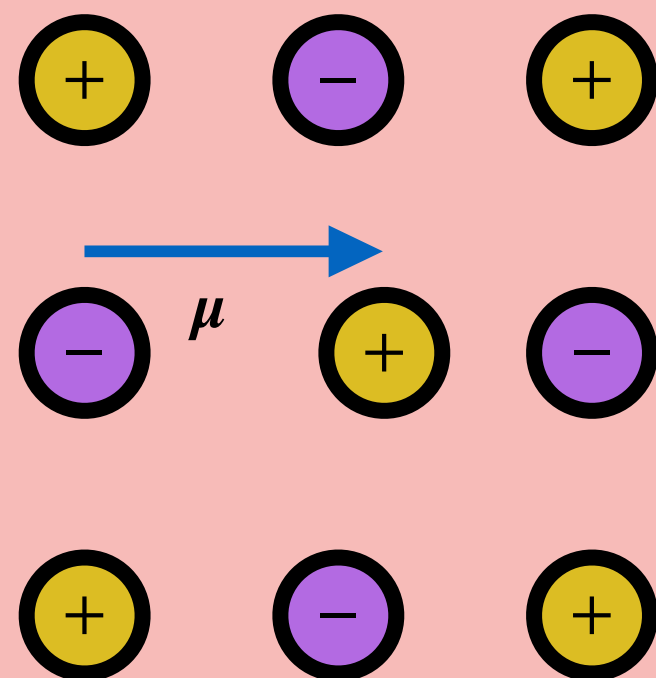
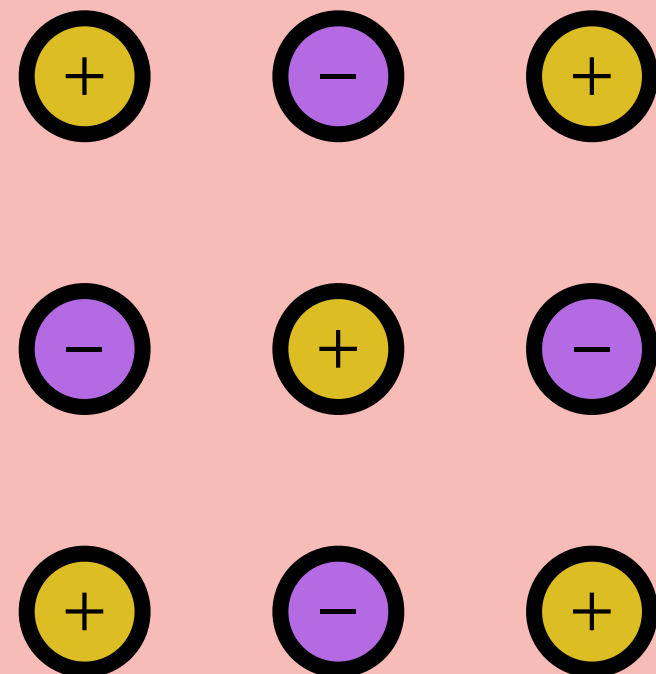
electronic
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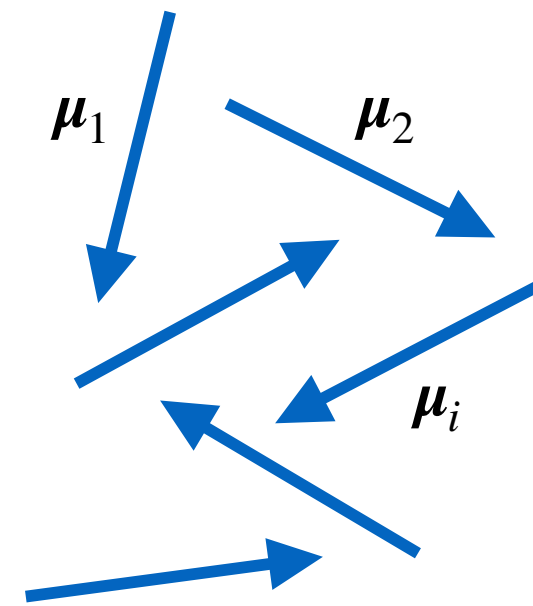
ionic
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$$\mu = 0$$

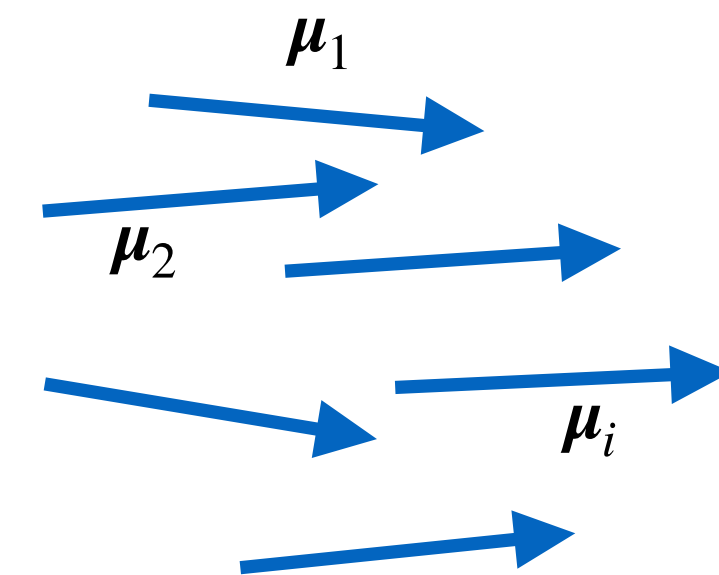


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orientation
polarisation



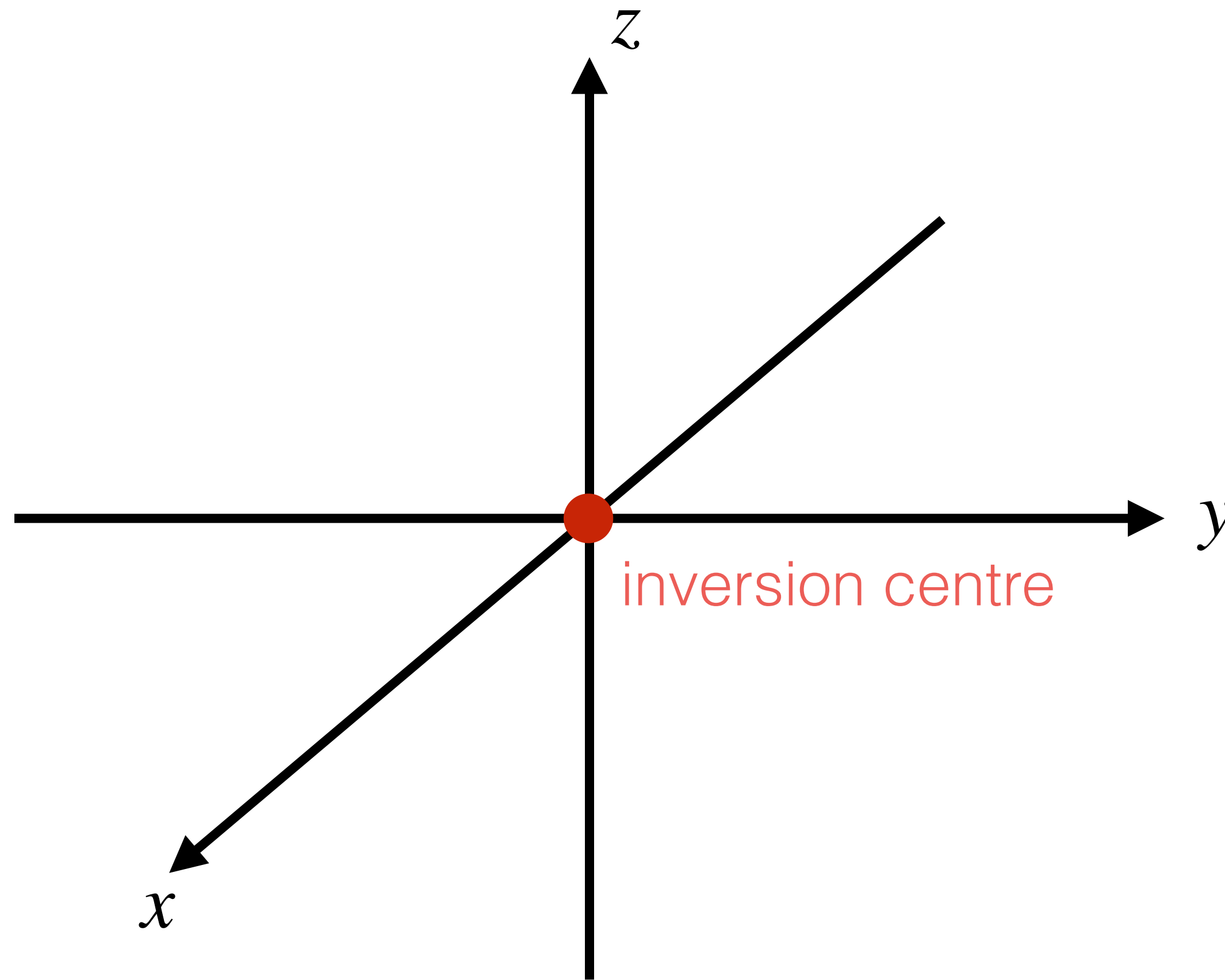
$$\mu = \sum_{i=1}^N \mu_i \simeq 0$$



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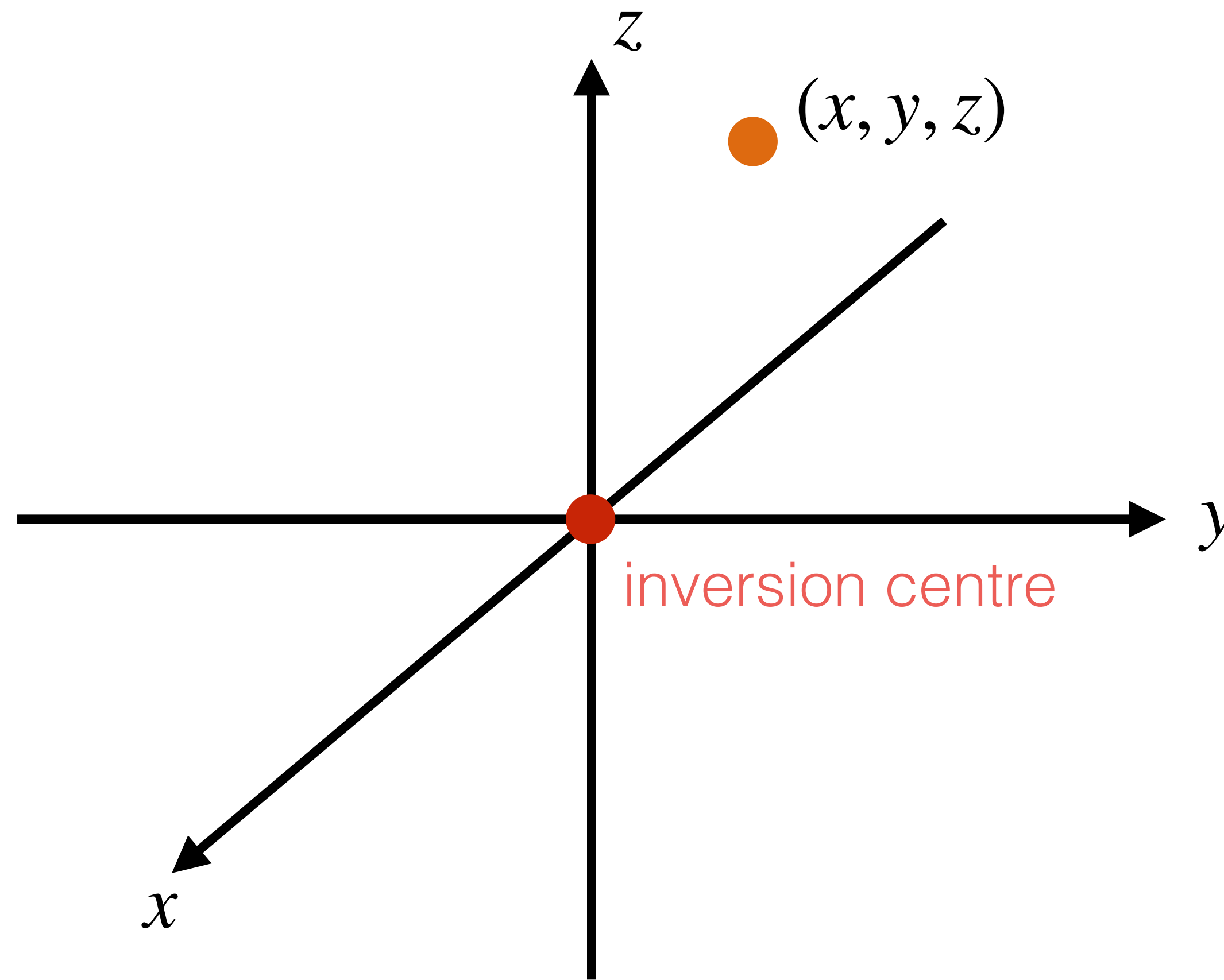
Centrosymmetric crystals

- A centrosymmetric crystals has an **inversion centre**



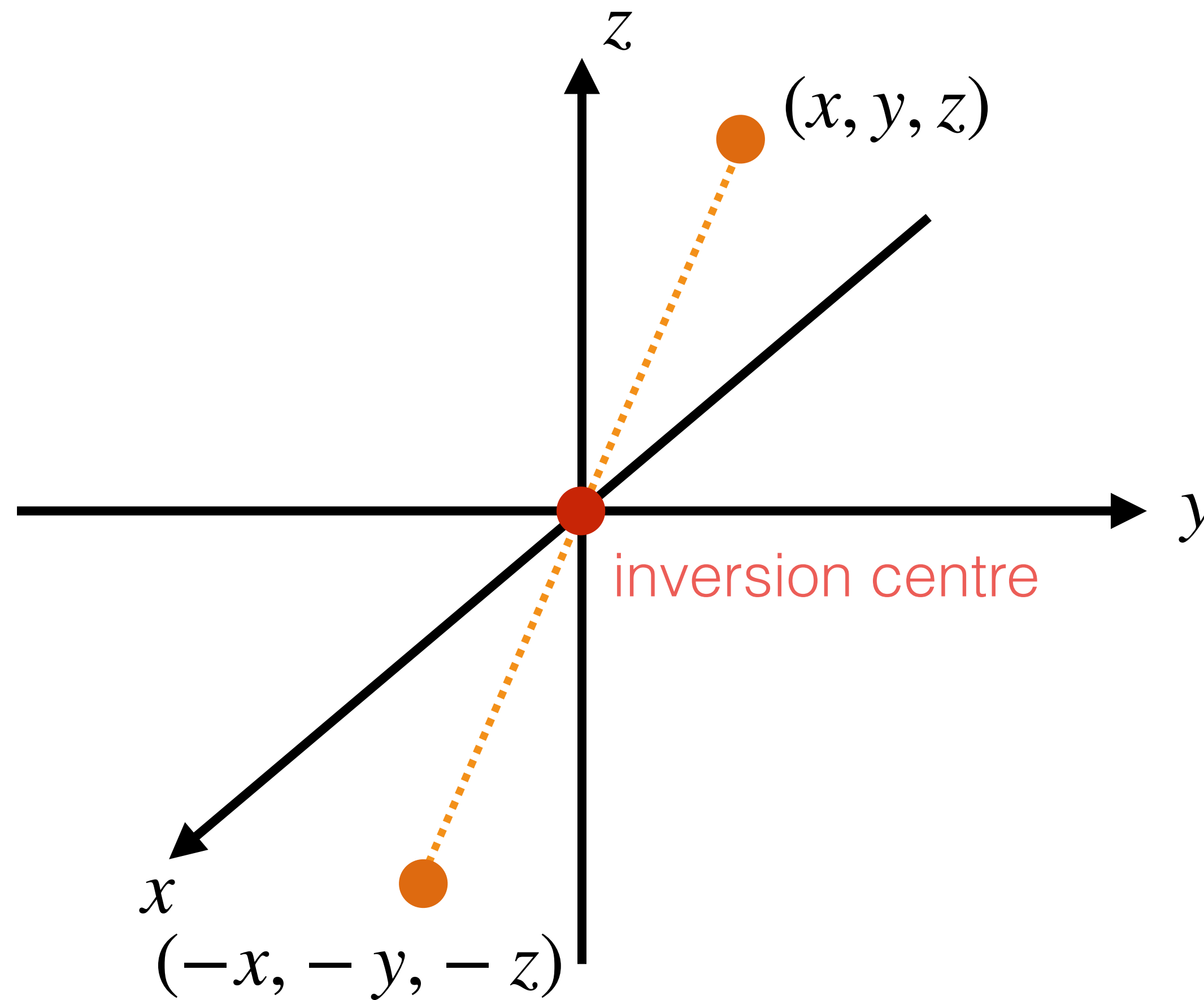
Centrosymmetric crystals

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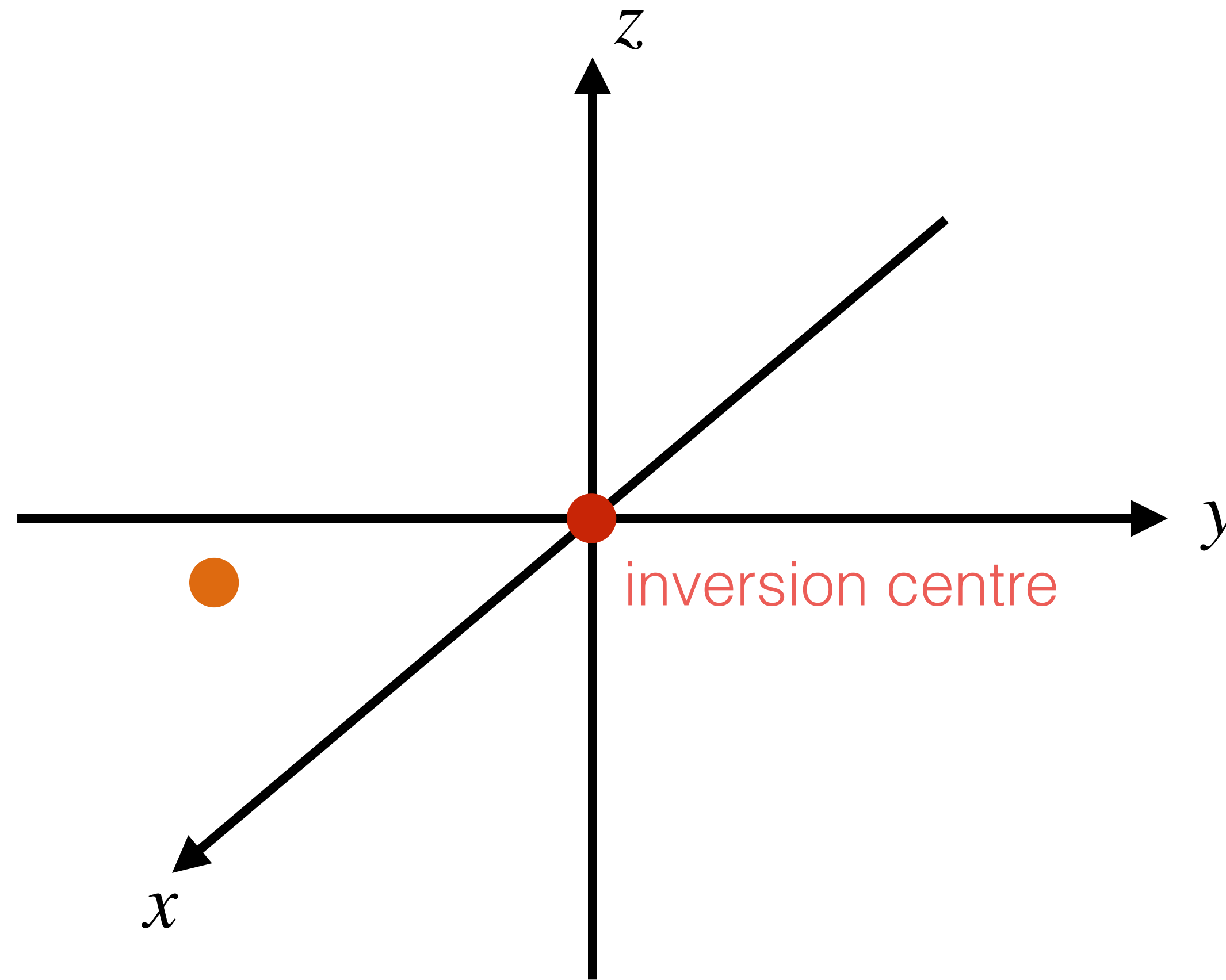
Centrosymmetric crystals

- A centrosymmetric crystals has an **inversion centre**



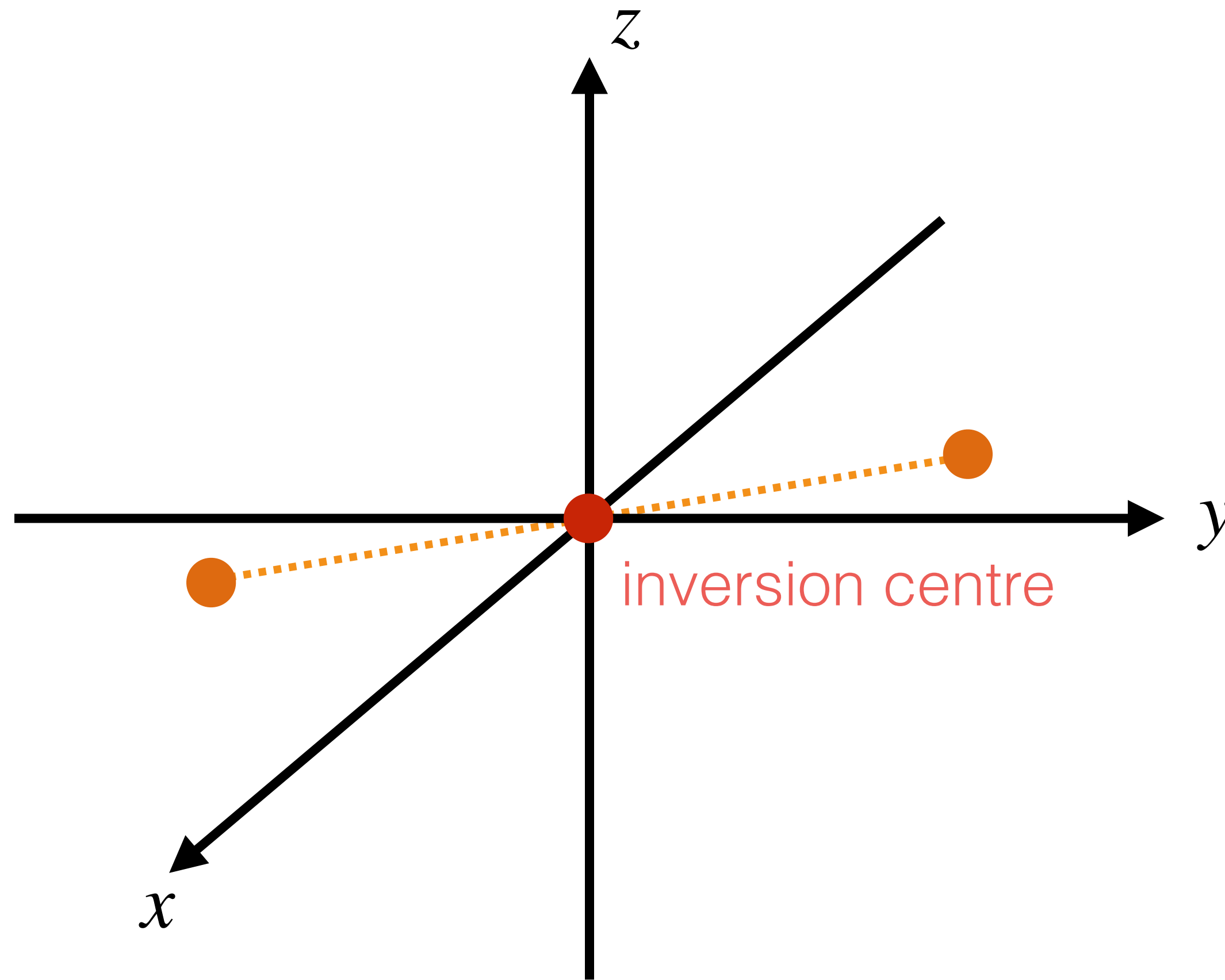
Centrosymmetric crystals

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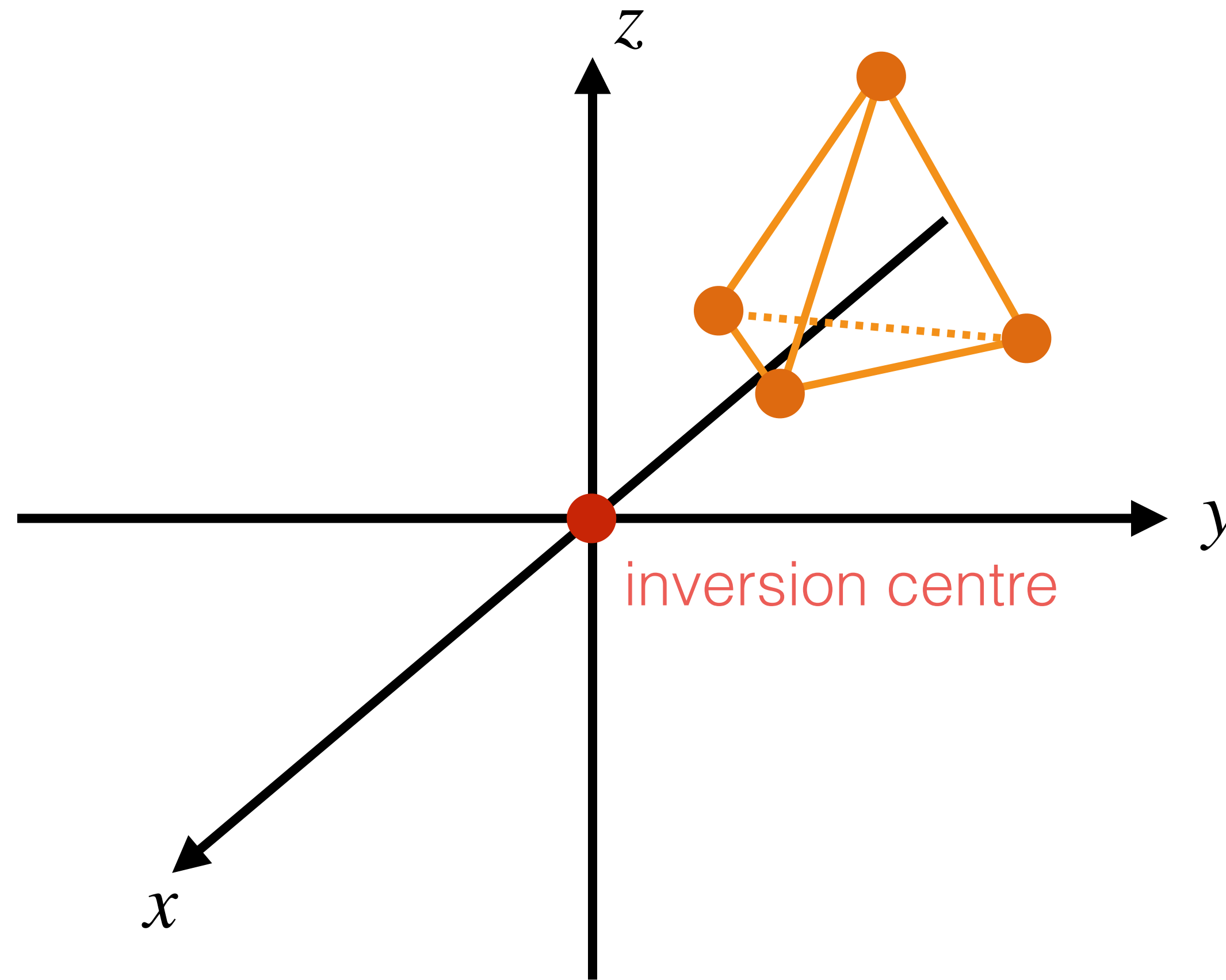
Centrosymmetric crystals

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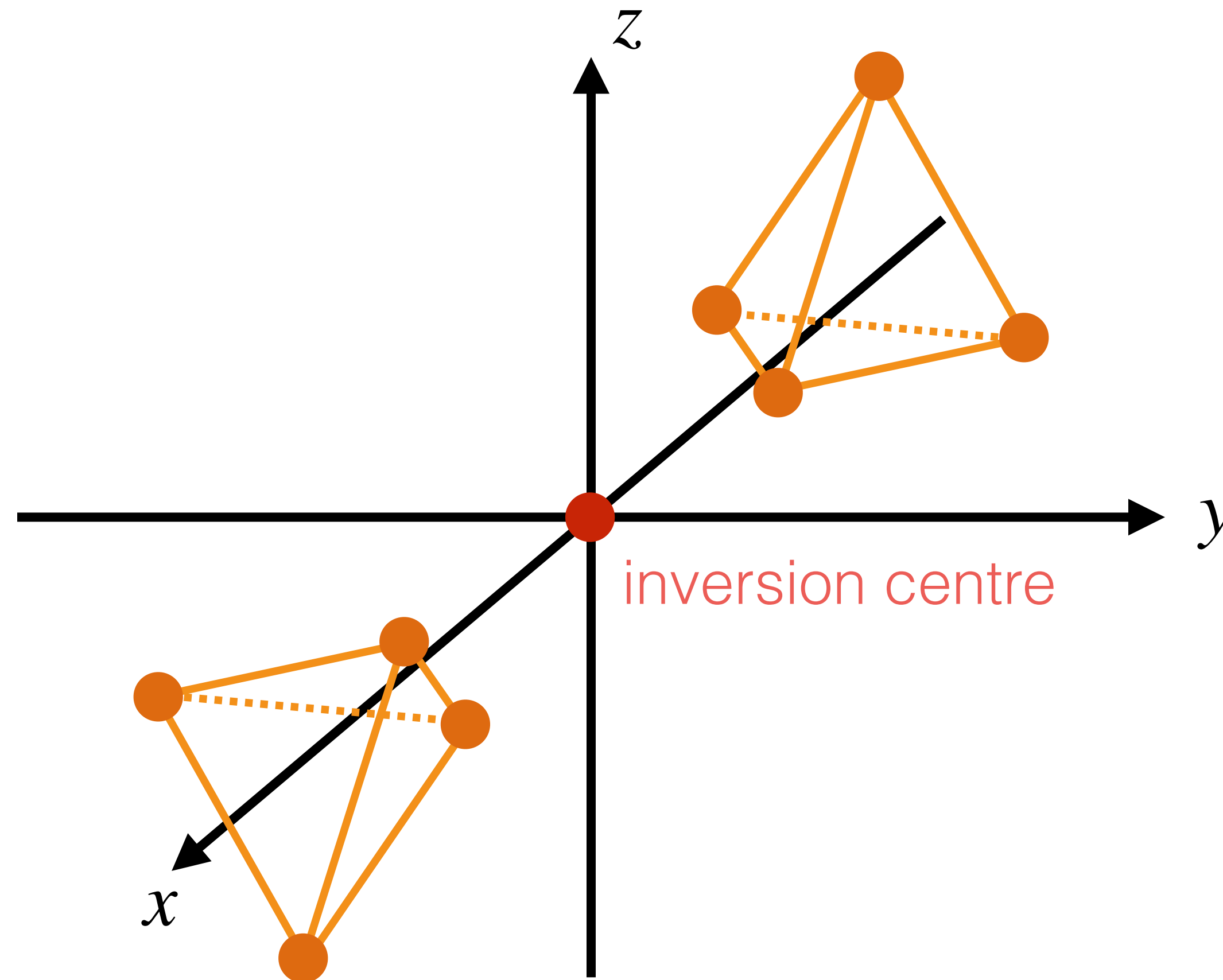
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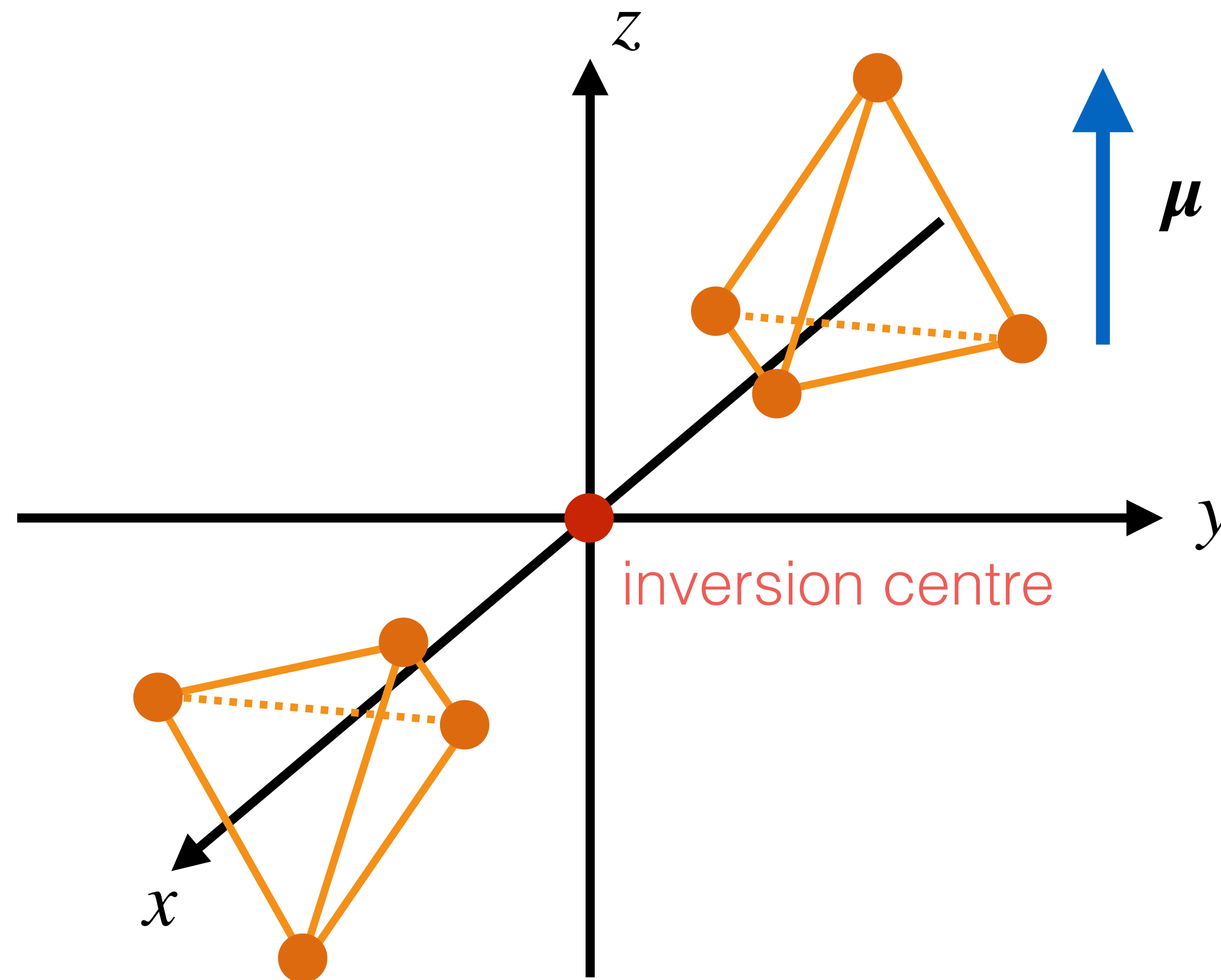
Centrosymmetric crystals

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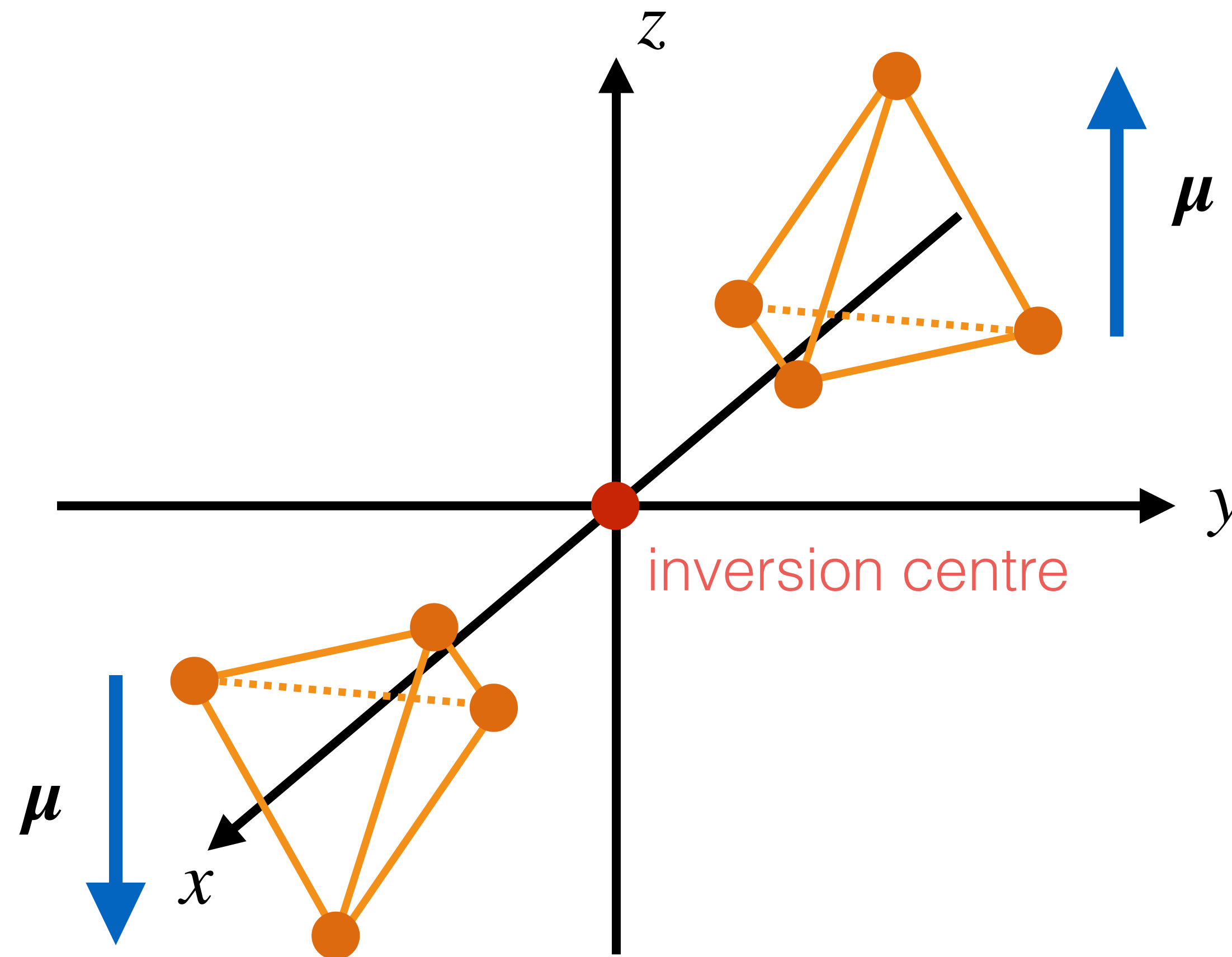
Centrosymmetric crystals

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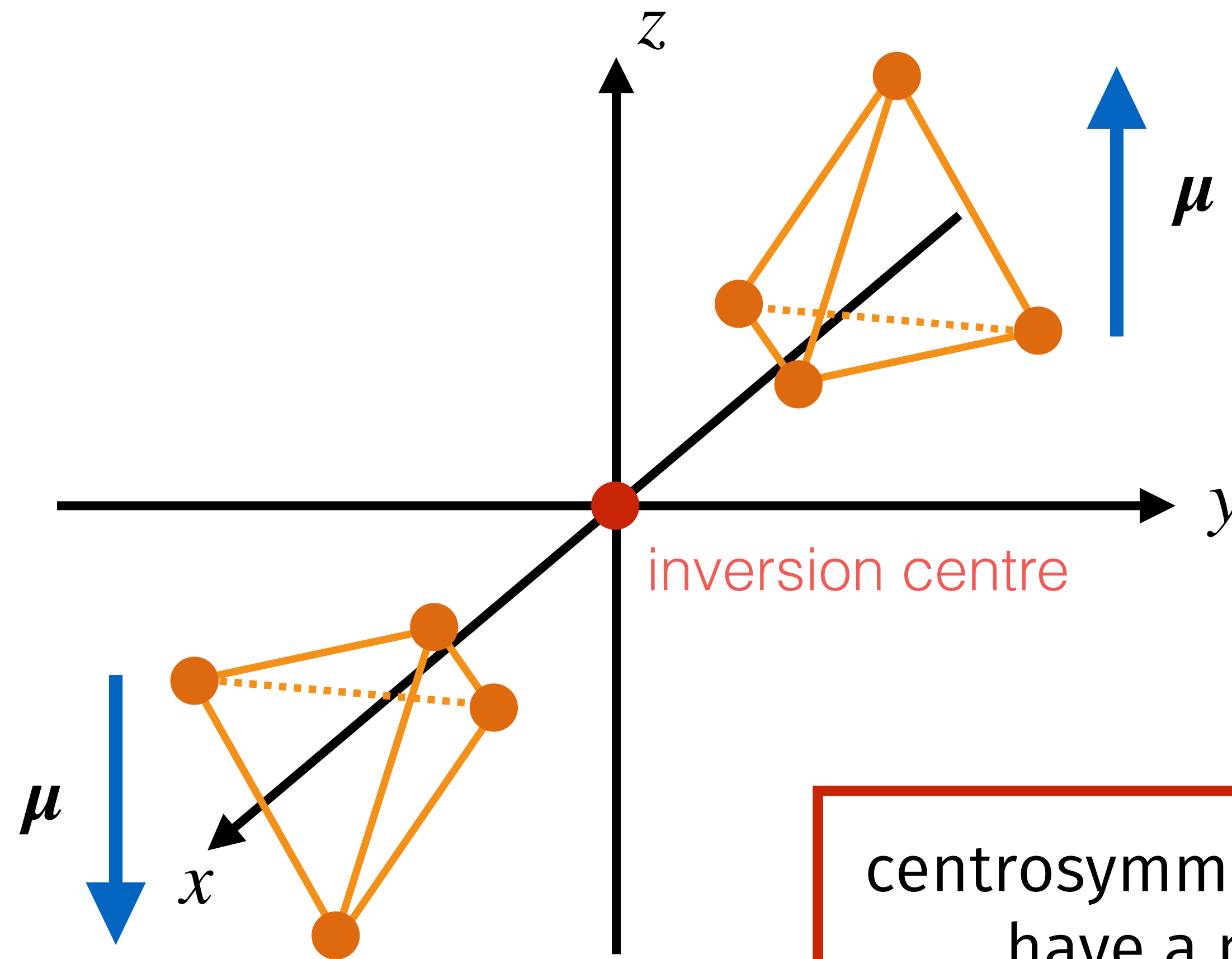
Centrosymmetric crystals

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Centrosymmetric crystals

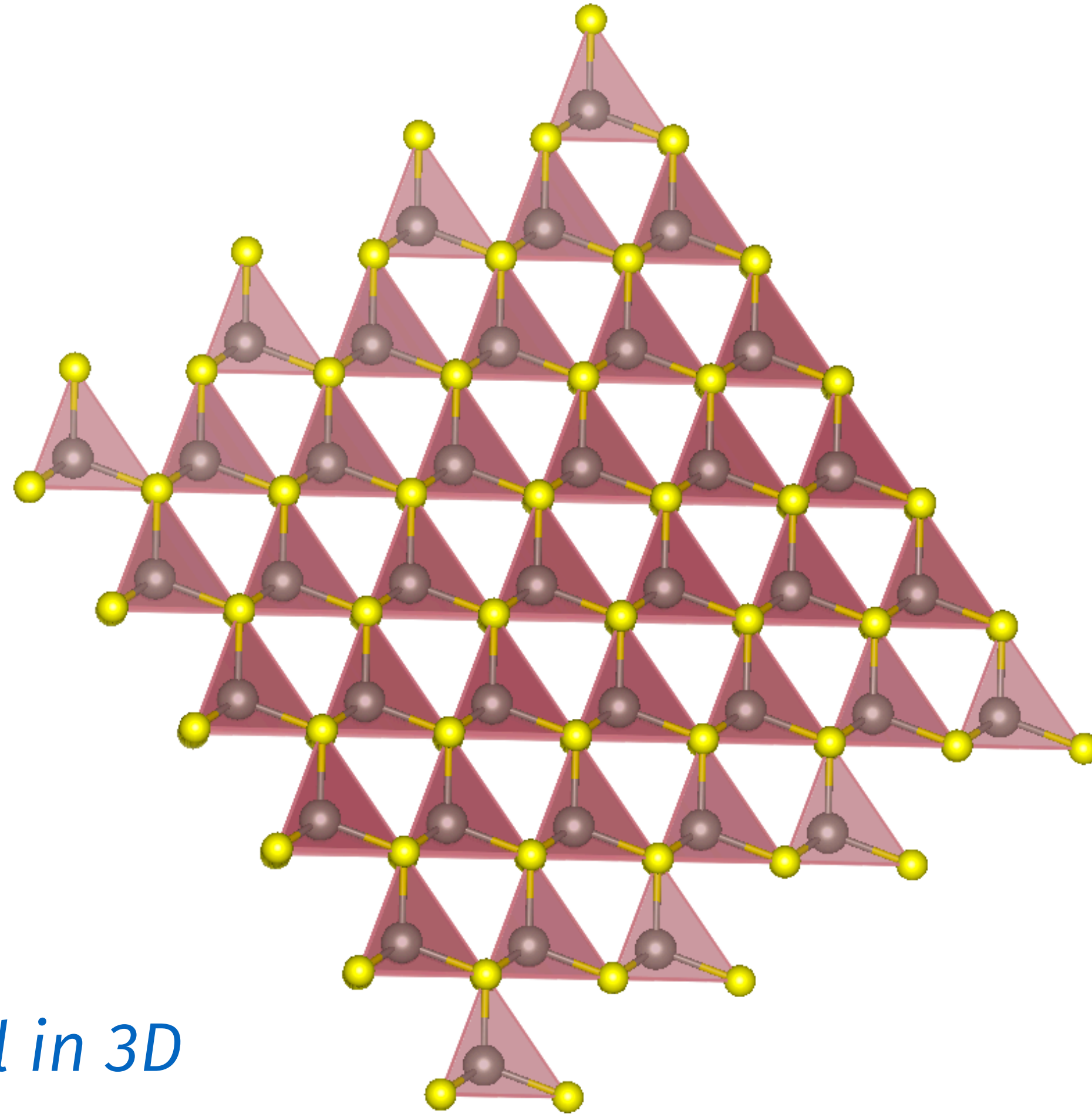
- A centrosymmetric crystals has an **inversion centre**



centrosymmetric crystals cannot have a net polarisation

Non-centrosymmetric crystals

- ▶ A non-centrosymmetric crystals does not have an **inversion centre**

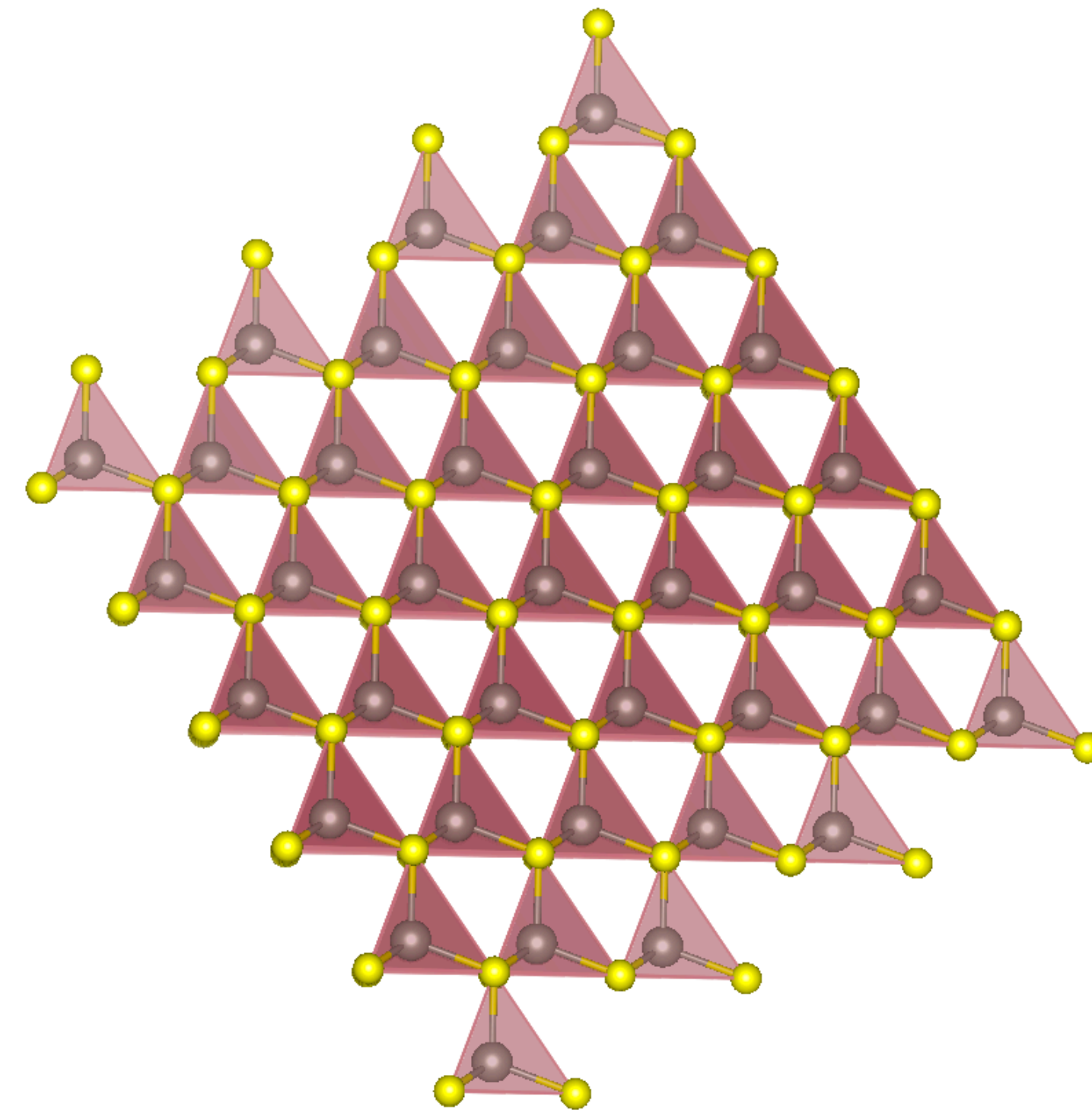
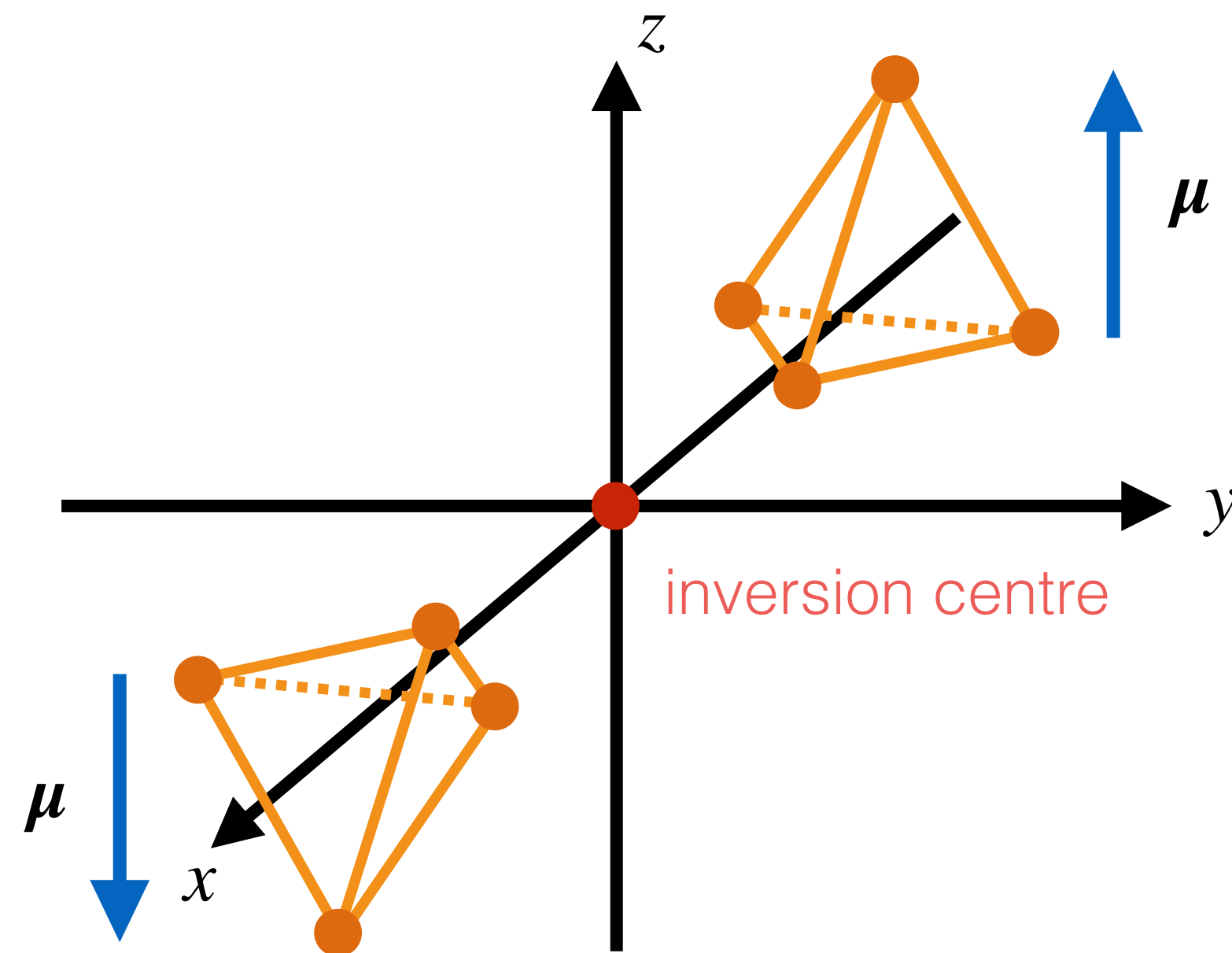


- ▶ ZnS (zinc blende)
- ▶ Face-centred cubic (fcc)
- ▶ Two-atom basis
- ▶ Course A: sphalerite

- ▶ *See structure model in 3D*

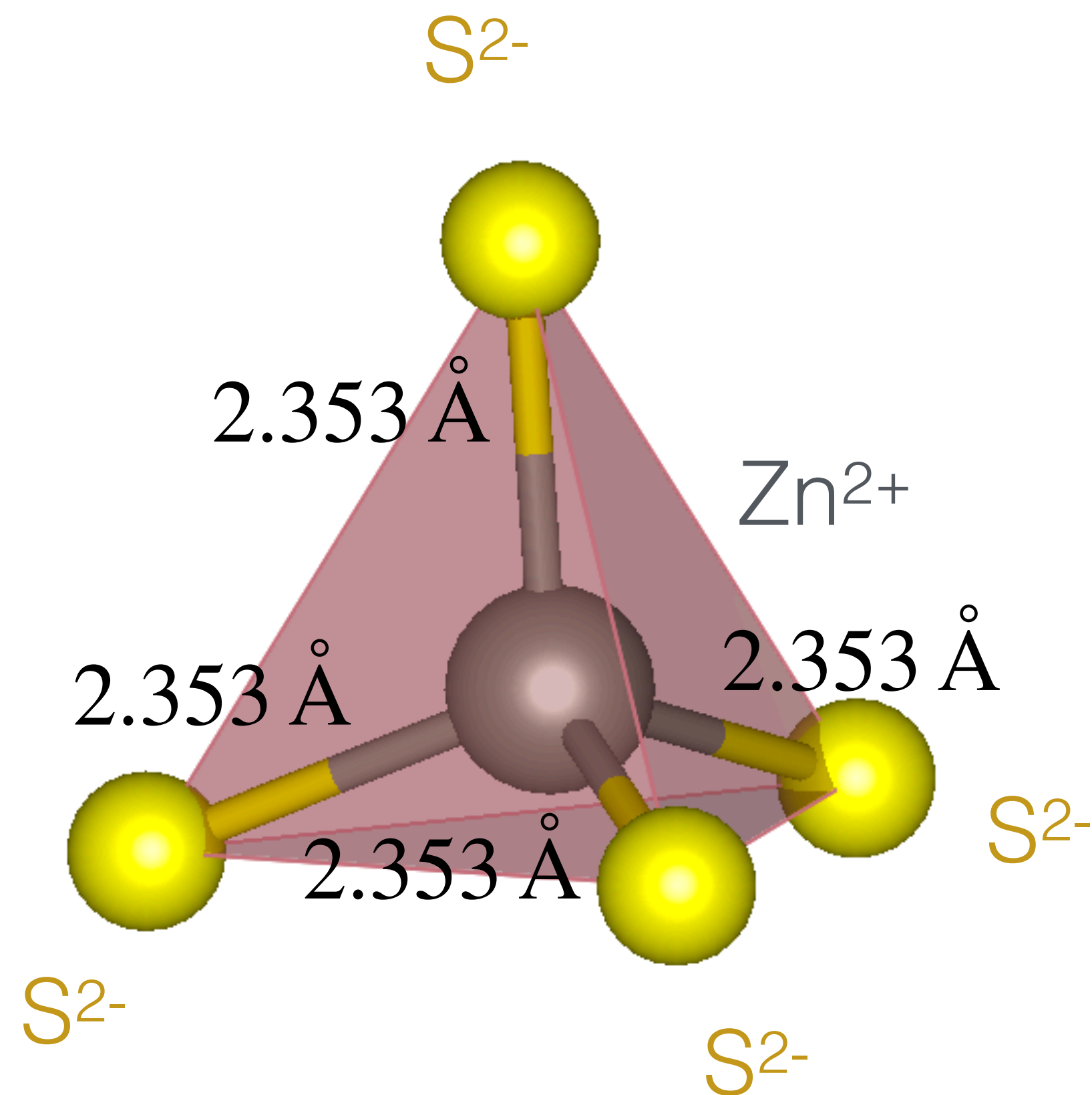
Non-centrosymmetric crystals: non-polar

- ▶ A non-centrosymmetric crystals does not have an **inversion centre**
- ▶ Are all non-centrosymmetric crystals polar?



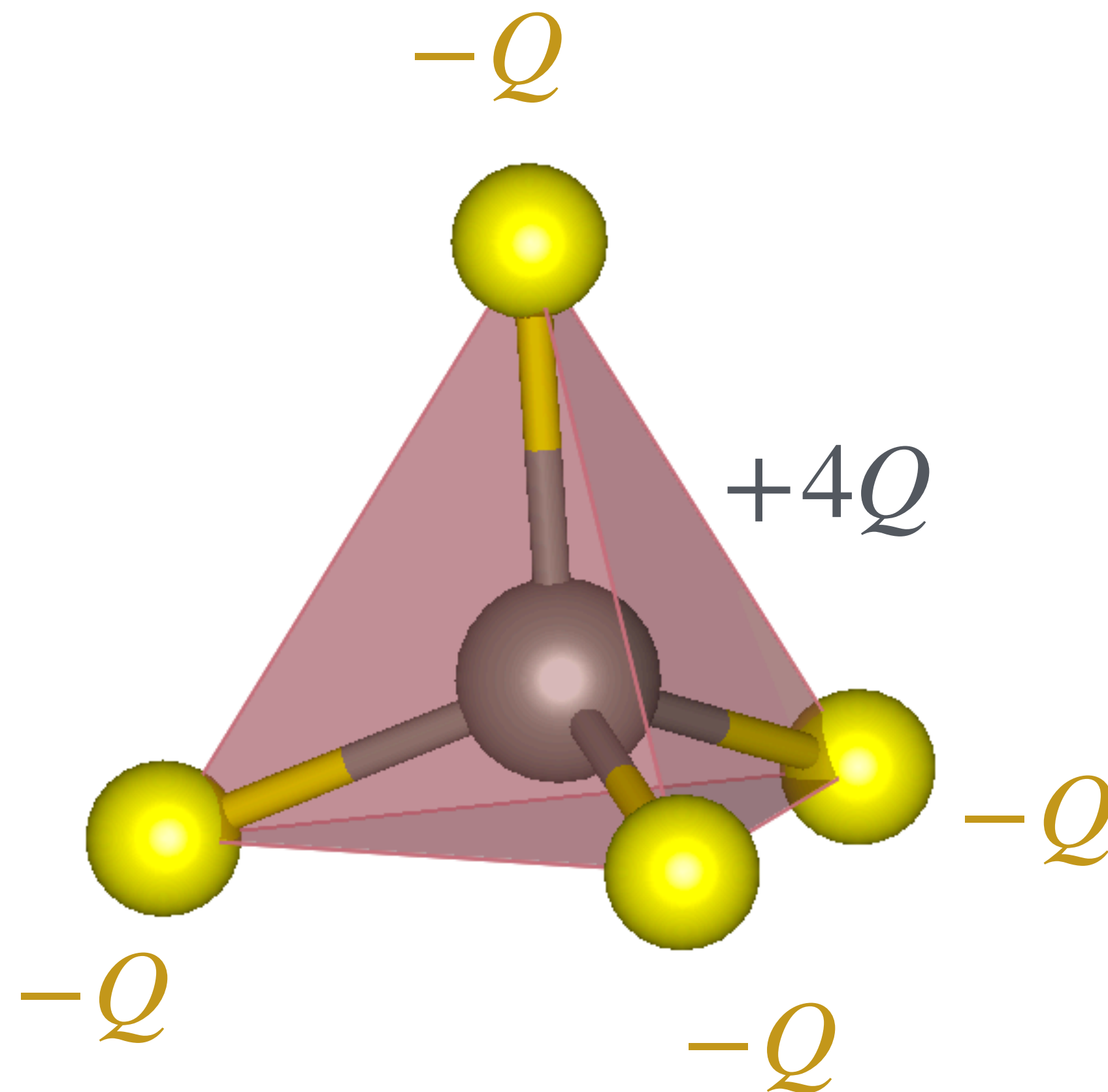
Non-centrosymmetric crystals: non-polar

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Non-centrosymmetric crystals: non-polar

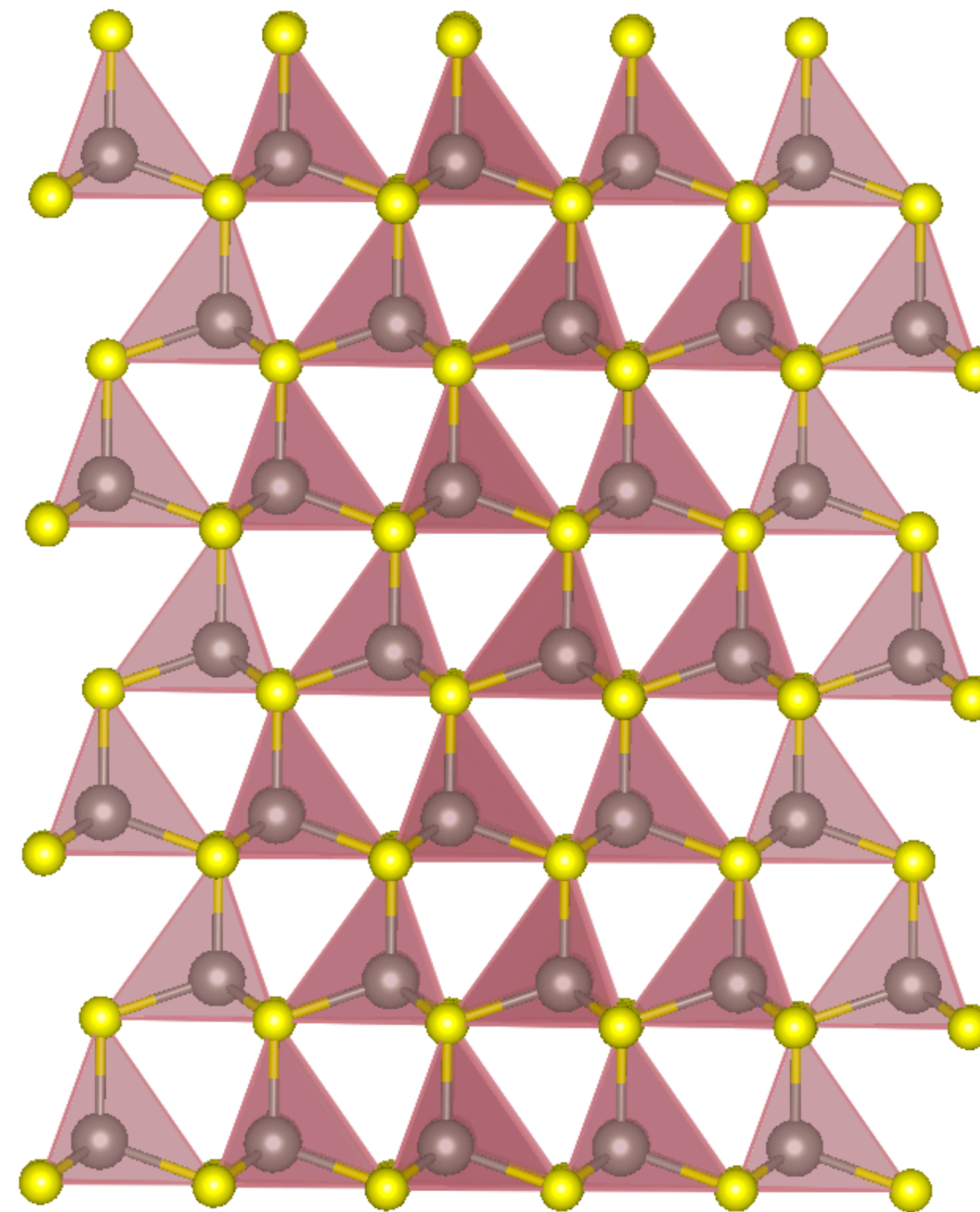
- A non-centrosymmetric crystals does not have an **inversion centre**
- Are all non-centrosymmetric crystals polar?



no net dipole

Non-centrosymmetric crystals: polar

- ▶ A non-centrosymmetric crystals does not have an **inversion centre**
- ▶ A non-centrosymmetric crystals can be **polar**

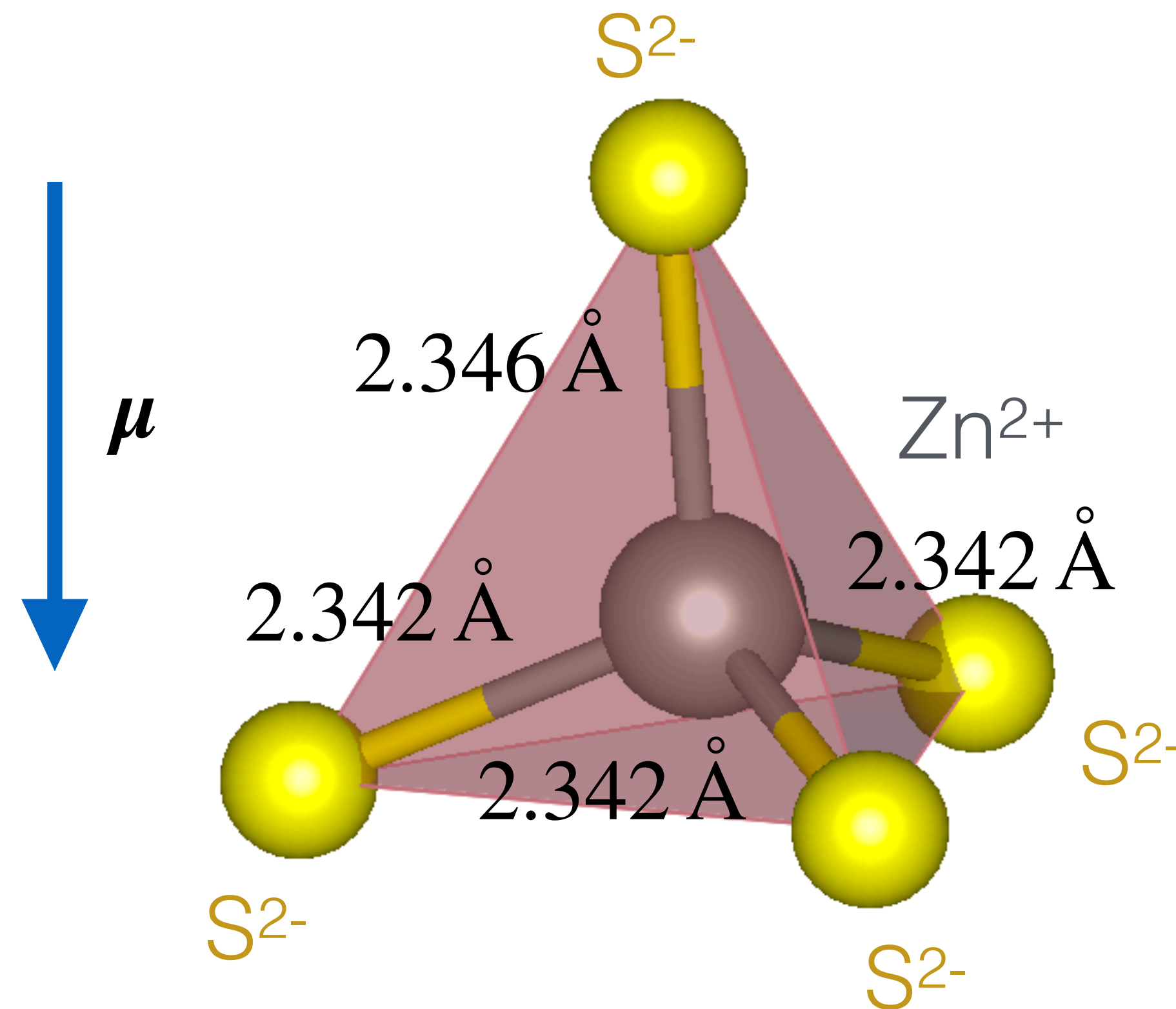


- ▶ ZnS (wurtzite)
- ▶ Hexagonal
- ▶ Four-atom basis
- ▶ Course A

- ▶ *See structure model in 3D*

Non-centrosymmetric crystals: non-polar

- ▶ A non-centrosymmetric crystals does not have an **inversion centre**
- ▶ A non-centrosymmetric crystals can be **polar**

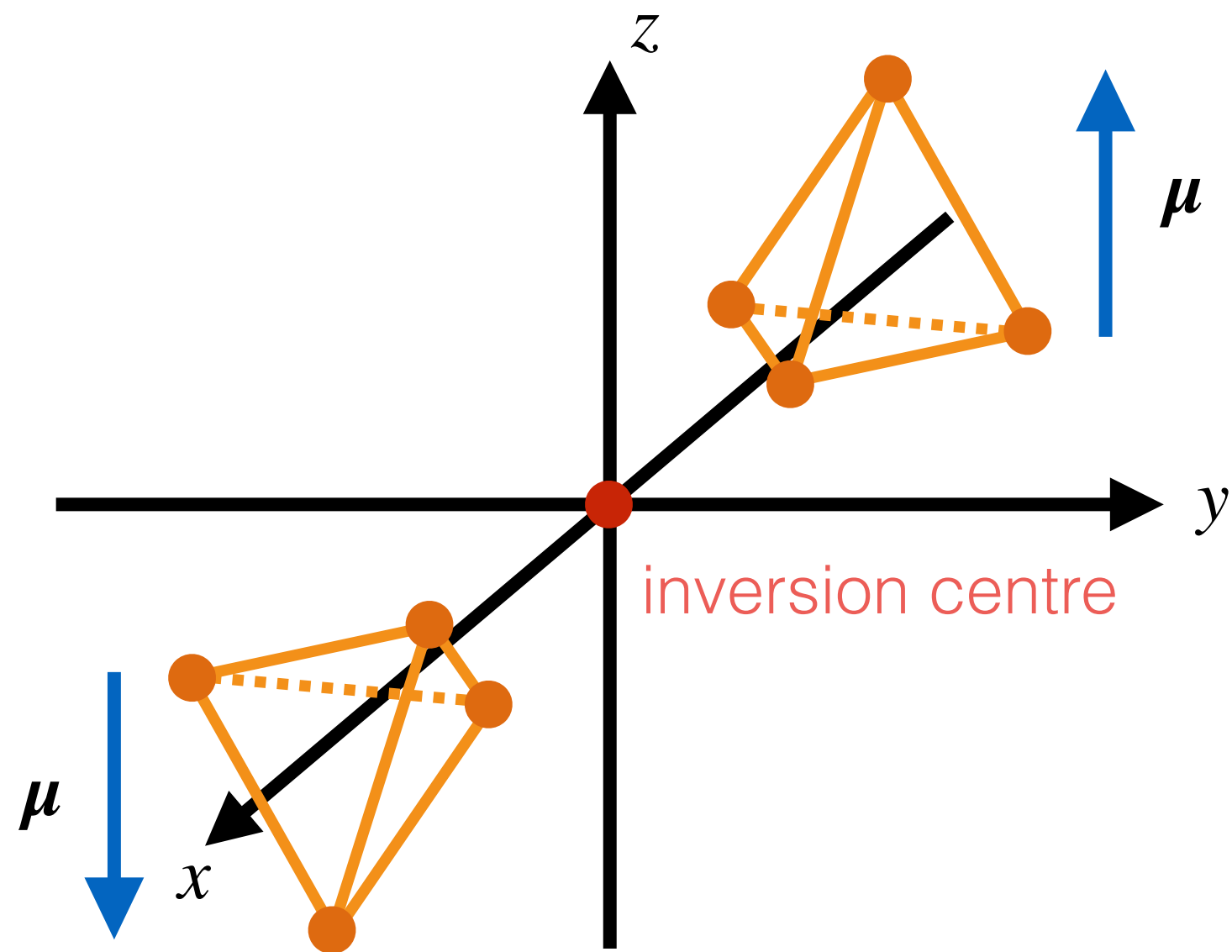


S: [Ne] 3s² 3p⁴

Zn: [Ar] 3d¹⁰ 4s²

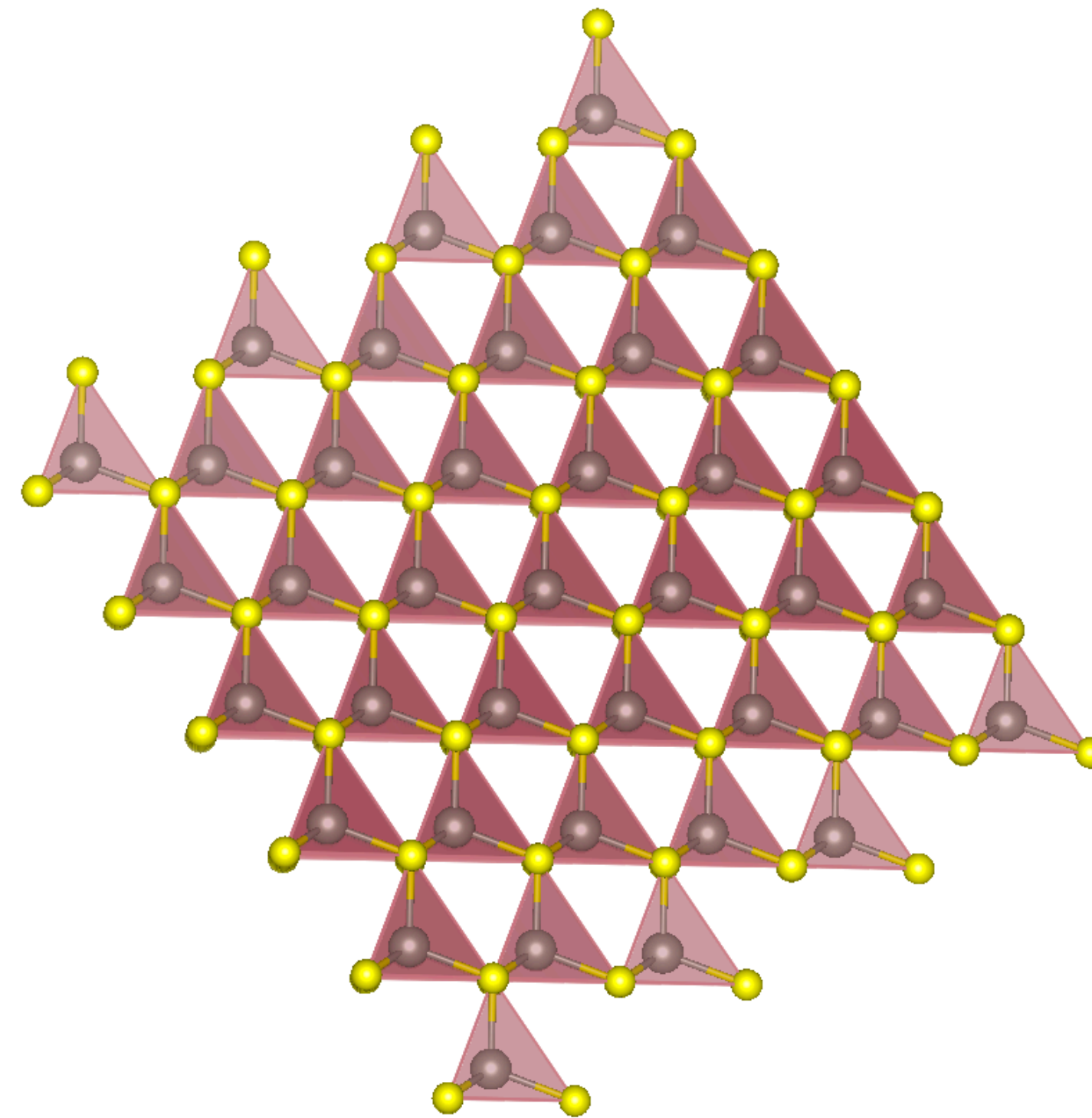
centrosymmetric crystal

non-polar

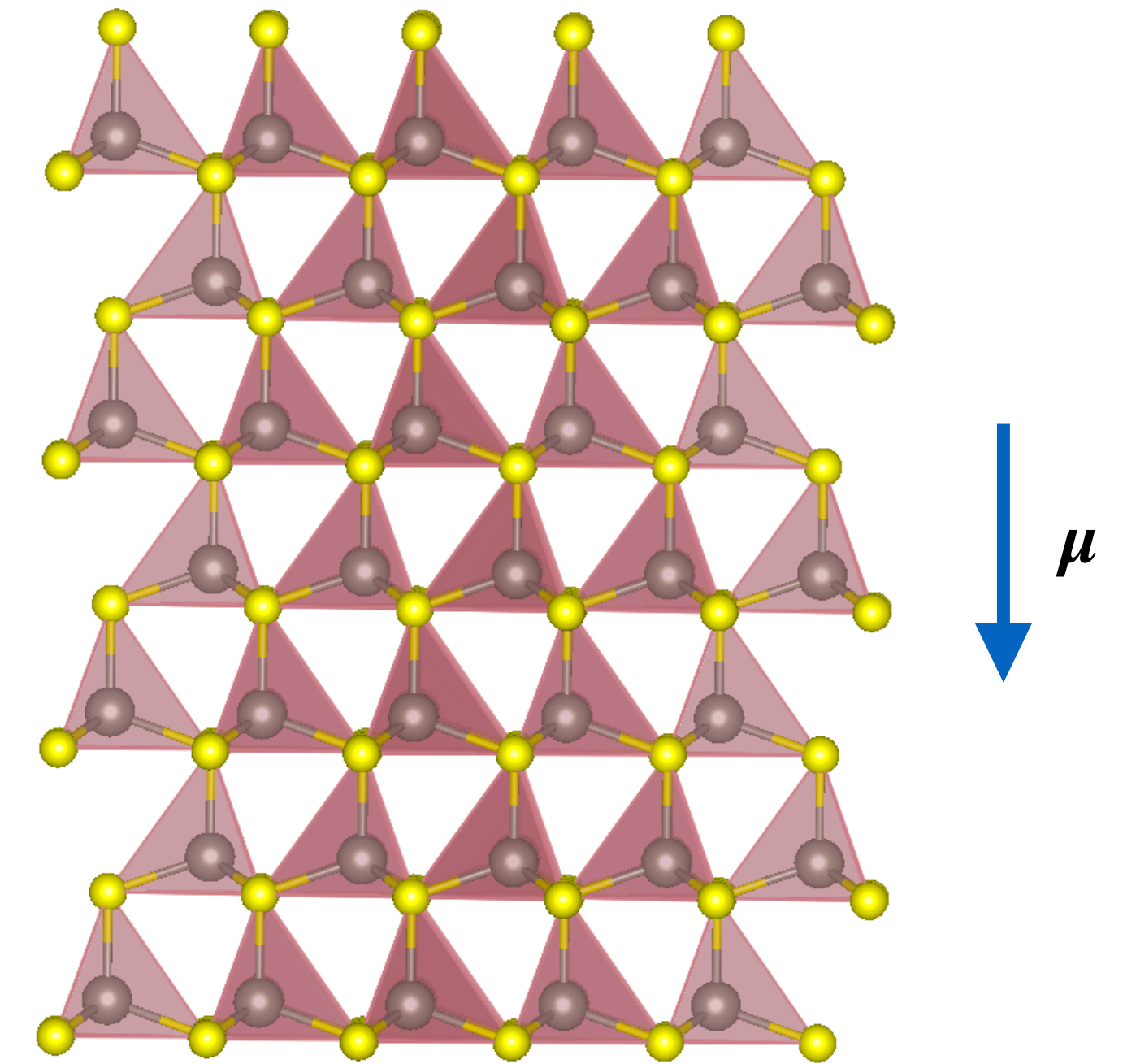


noncentrosymmetric crystal

non-polar

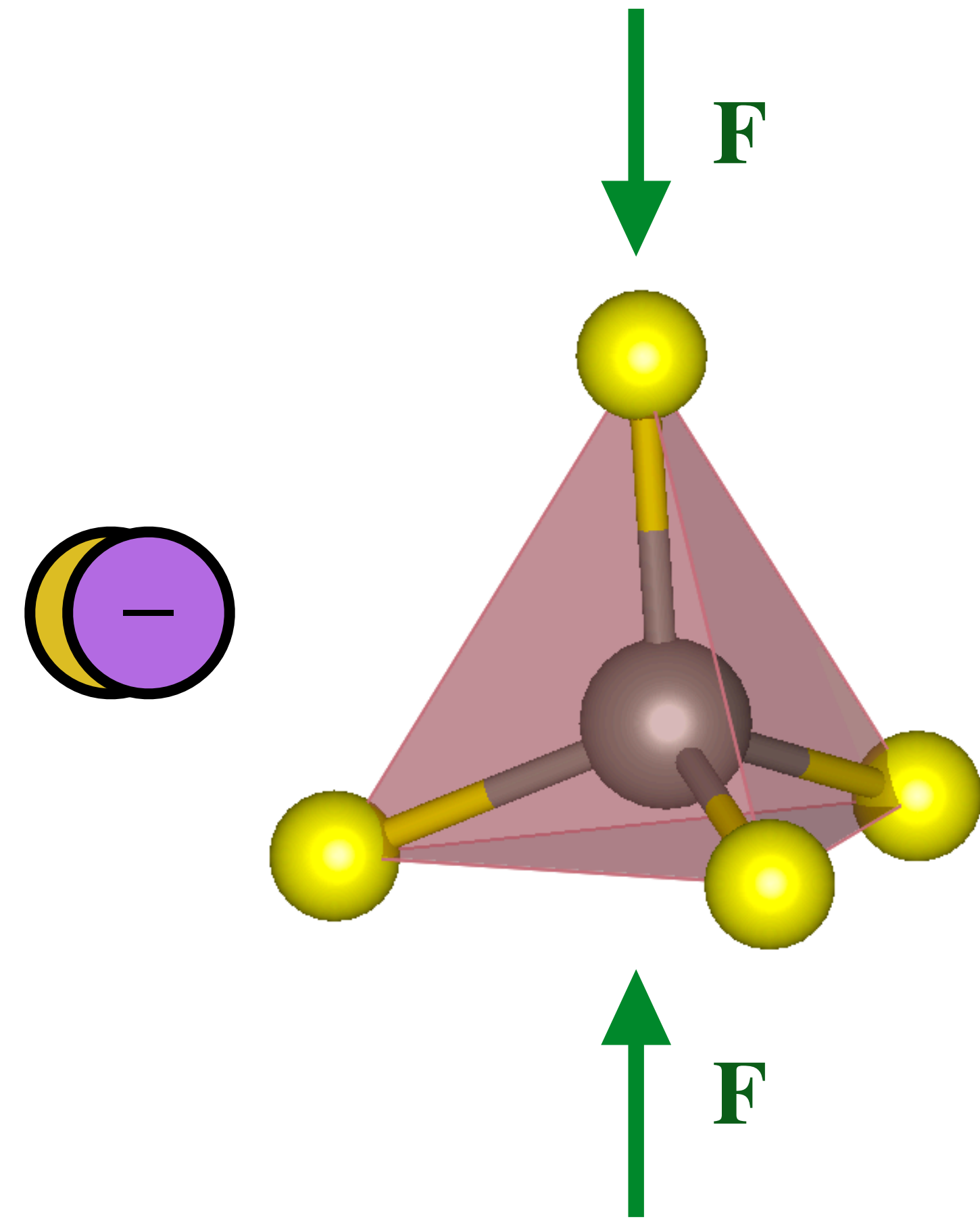
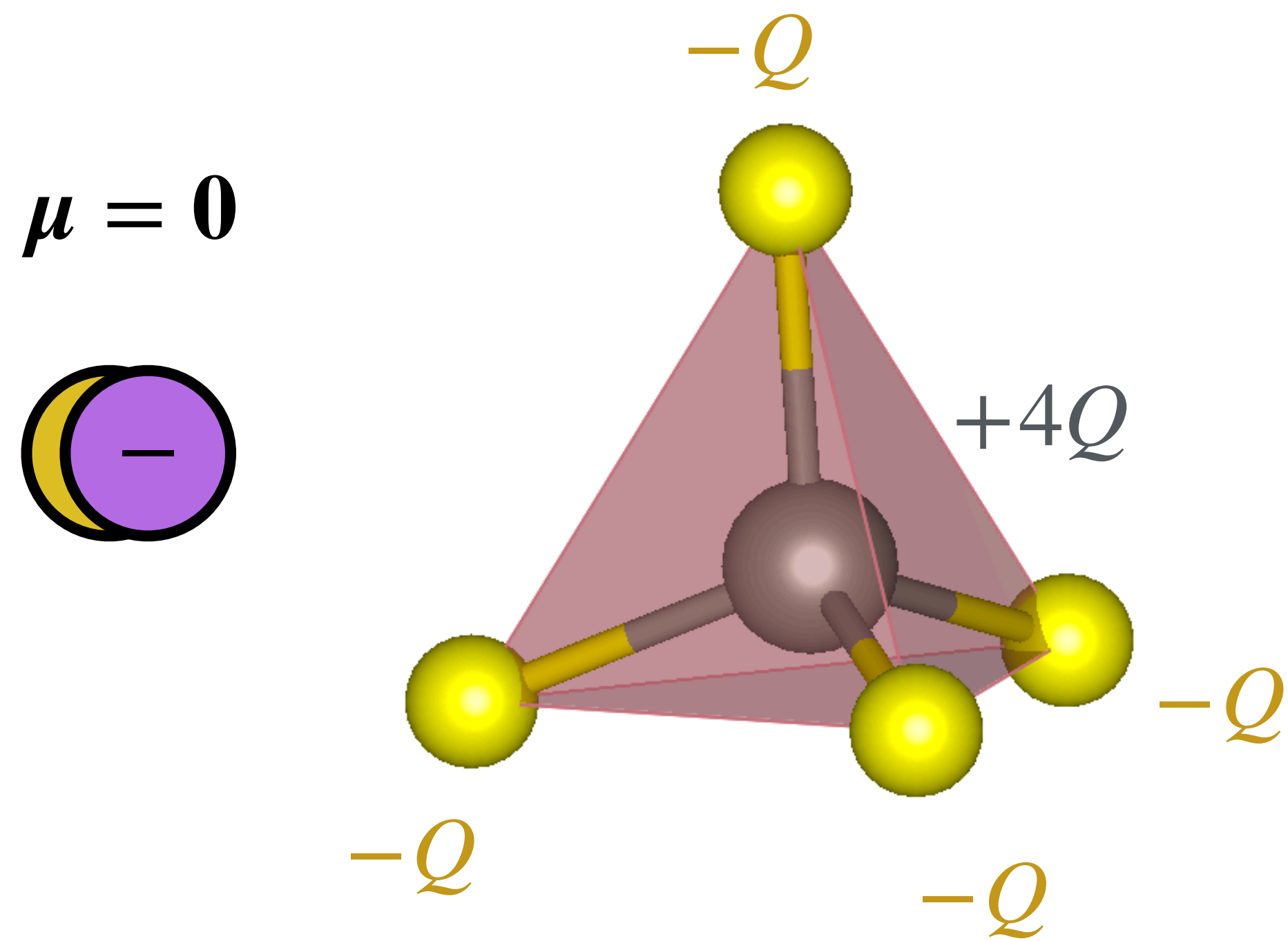


polar



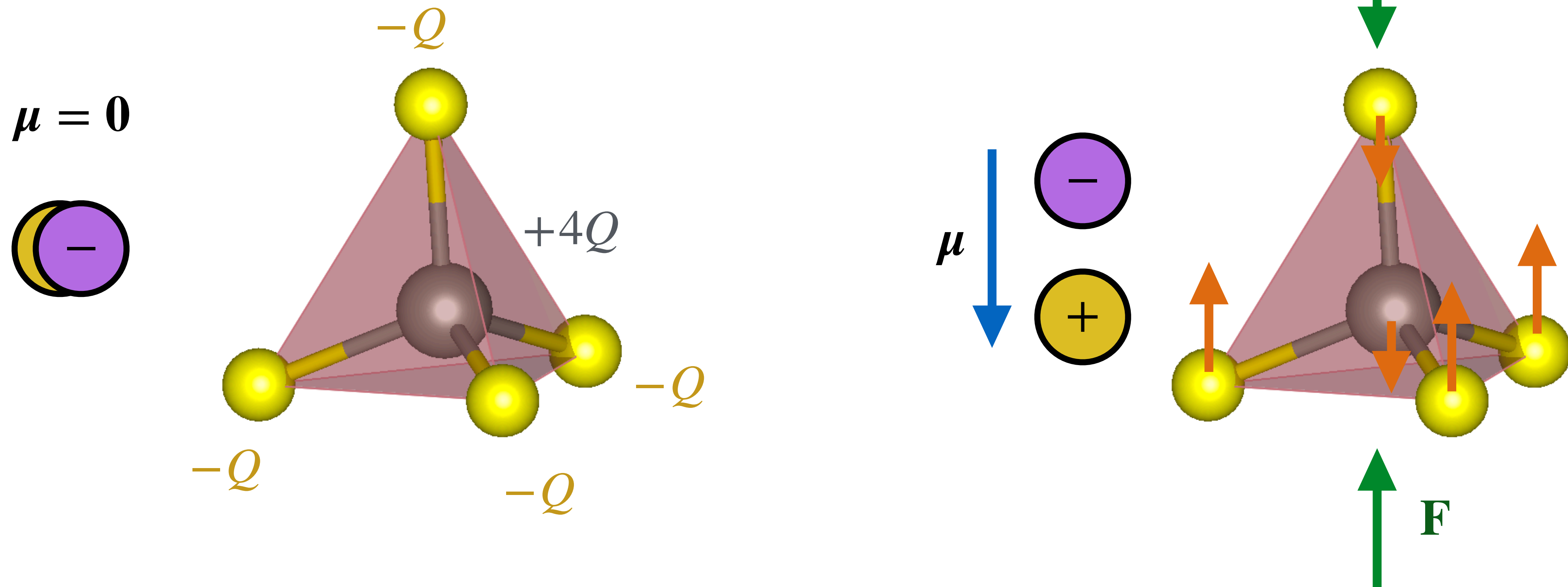
Piezoelectricity

- Piezoelectricity: dipole moment change due to the application of stress



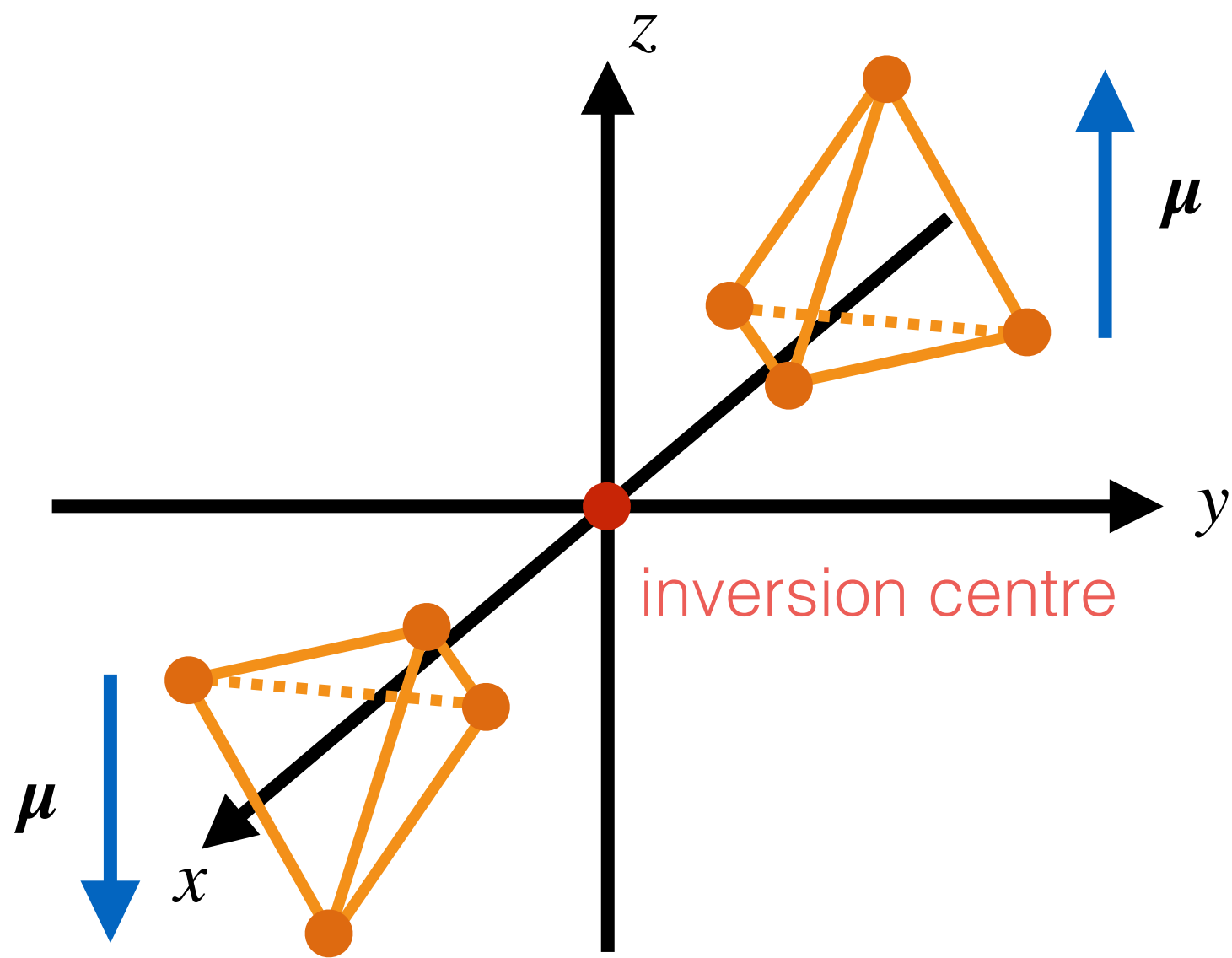
Piezoelectricity

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centrosymmetric crystal

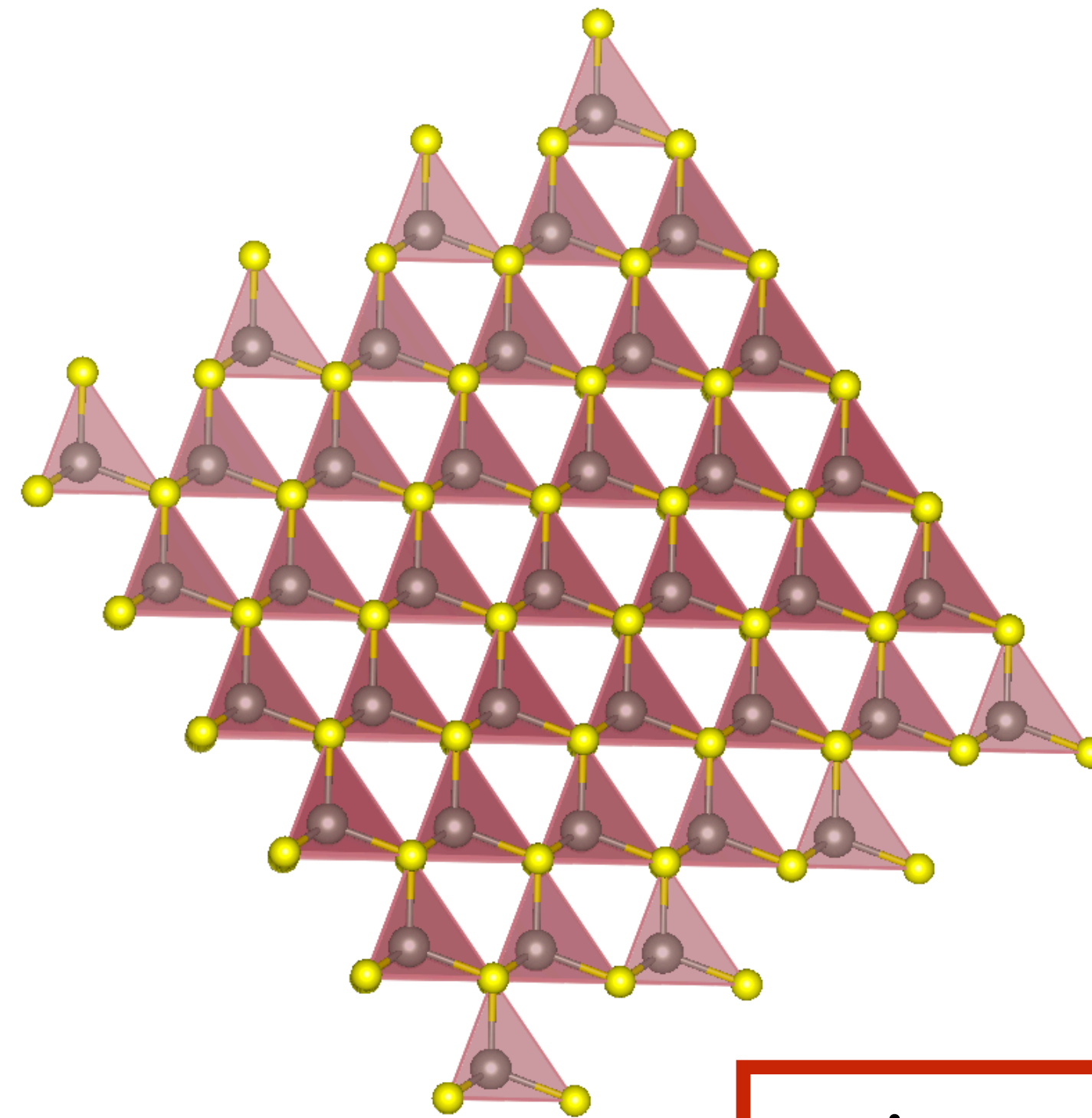
non-polar



no piezoelectricity

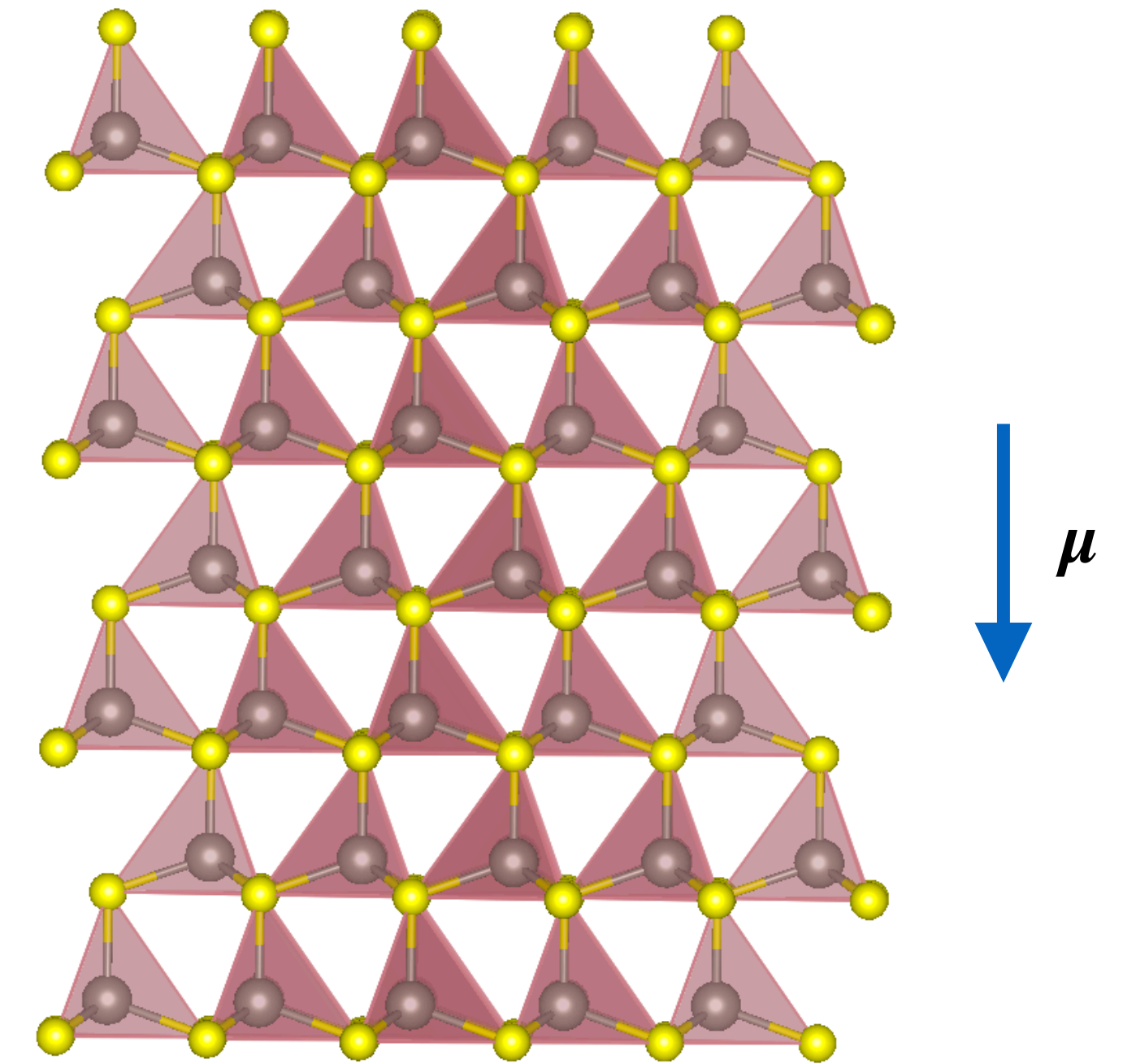
noncentrosymmetric crystal

non-polar



piezoelectricity*

polar



* Cubic crystal class 432 exception

Piezoelectricity

- *See discussion of piezoelectricity in rectangular prism*

$$\Delta V = \frac{dT L}{\epsilon}$$

ΔV : change in potential [V]

d : piezoelectric coefficient [C N⁻¹]

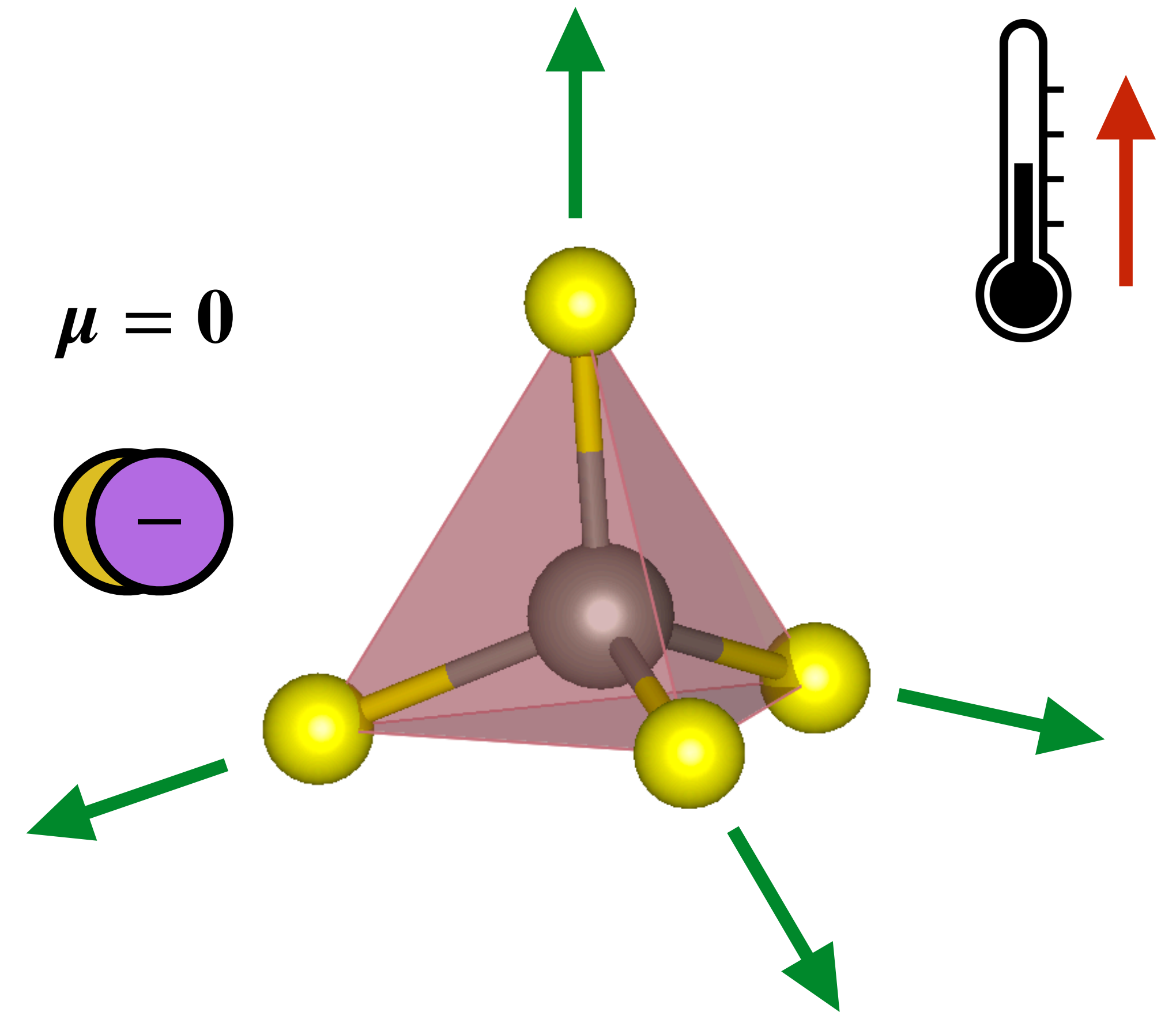
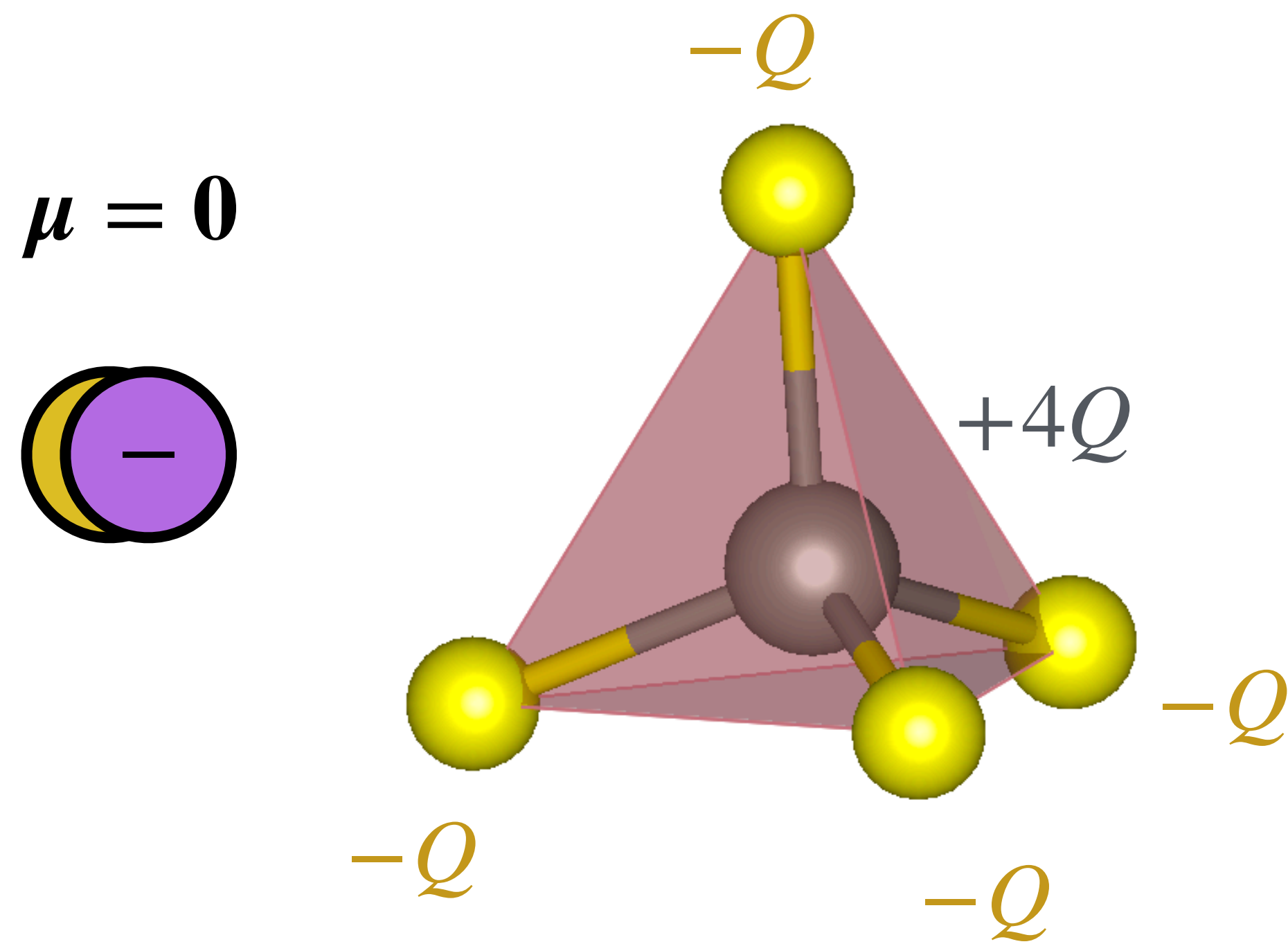
T : stress [N m⁻²]

L : length of prism [m]

ϵ : permittivity [F m⁻¹ = C V⁻¹ m⁻¹]

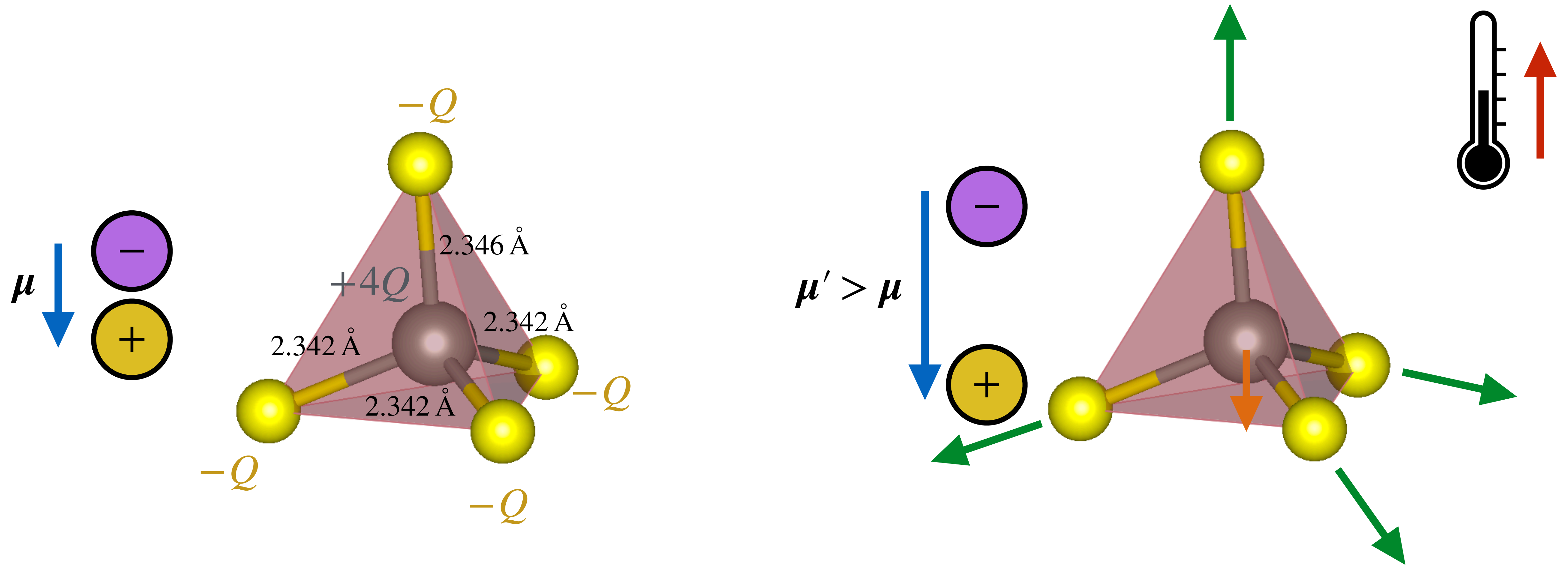
Pyroelectricity

- Pyroelectricity: dipole moment change due to temperature change



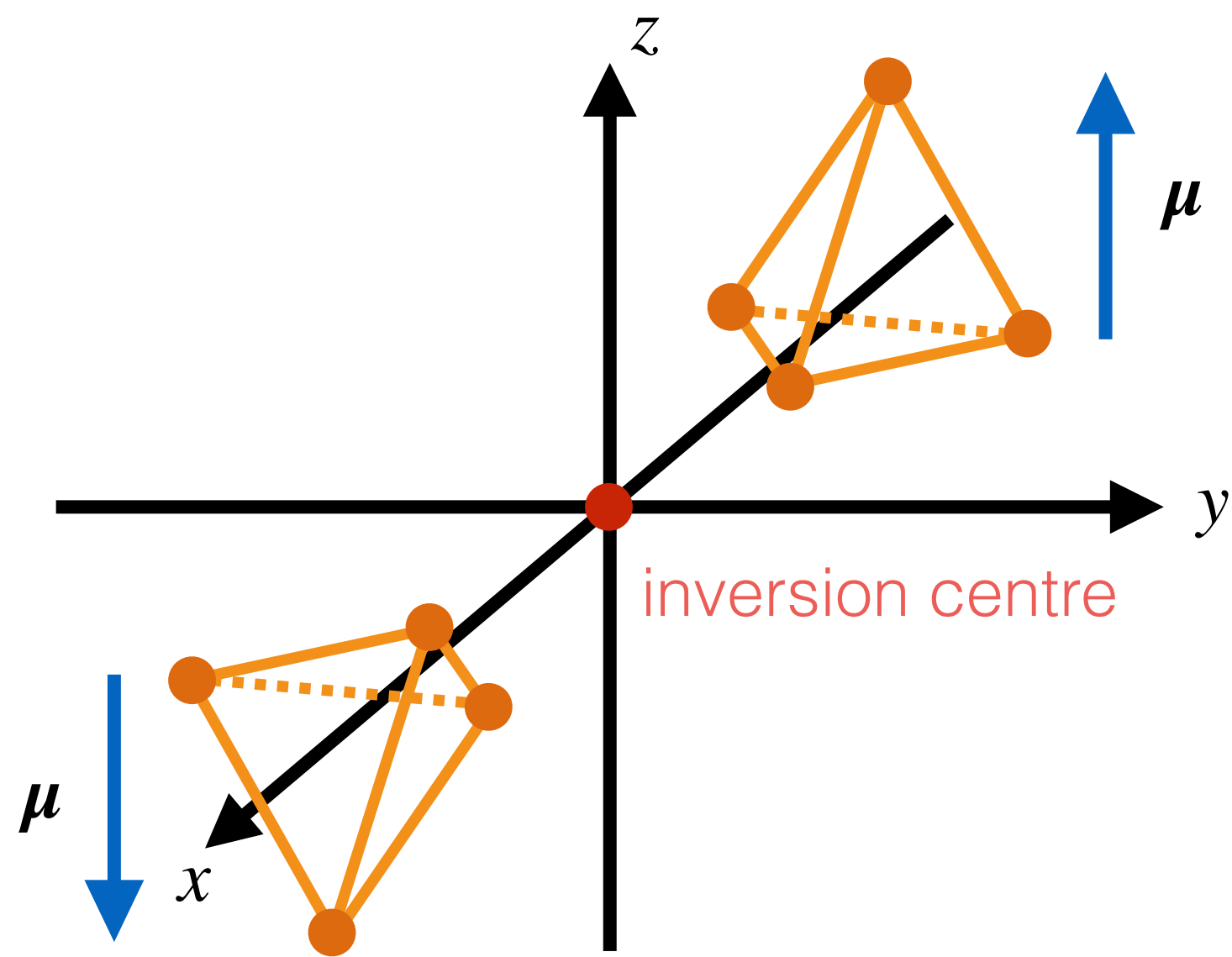
Pyroelectricity

- Pyroelectricity: dipole moment change due to temperature change



**centrosymmetric
crystal**

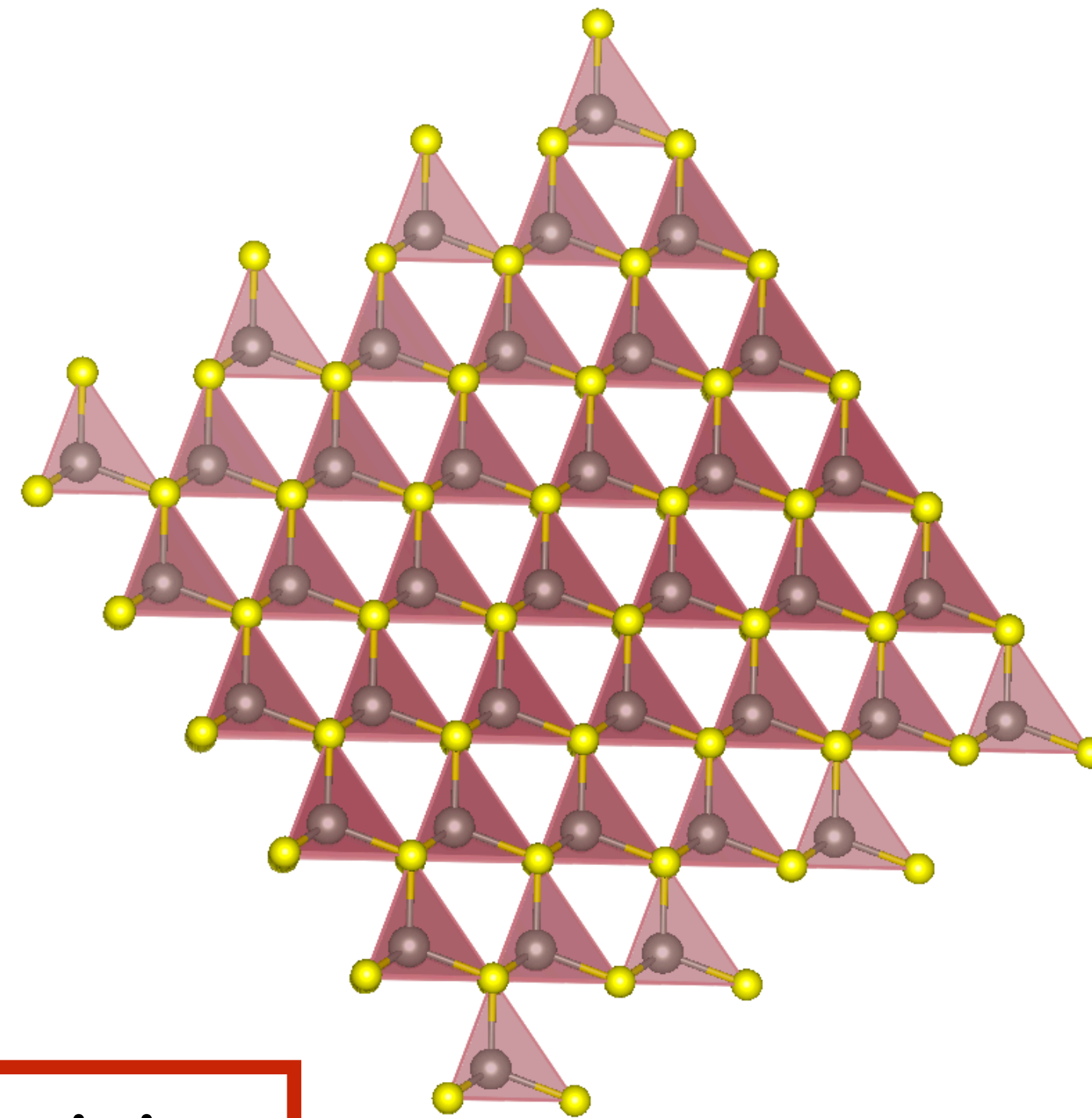
non-polar



no pyroelectricity

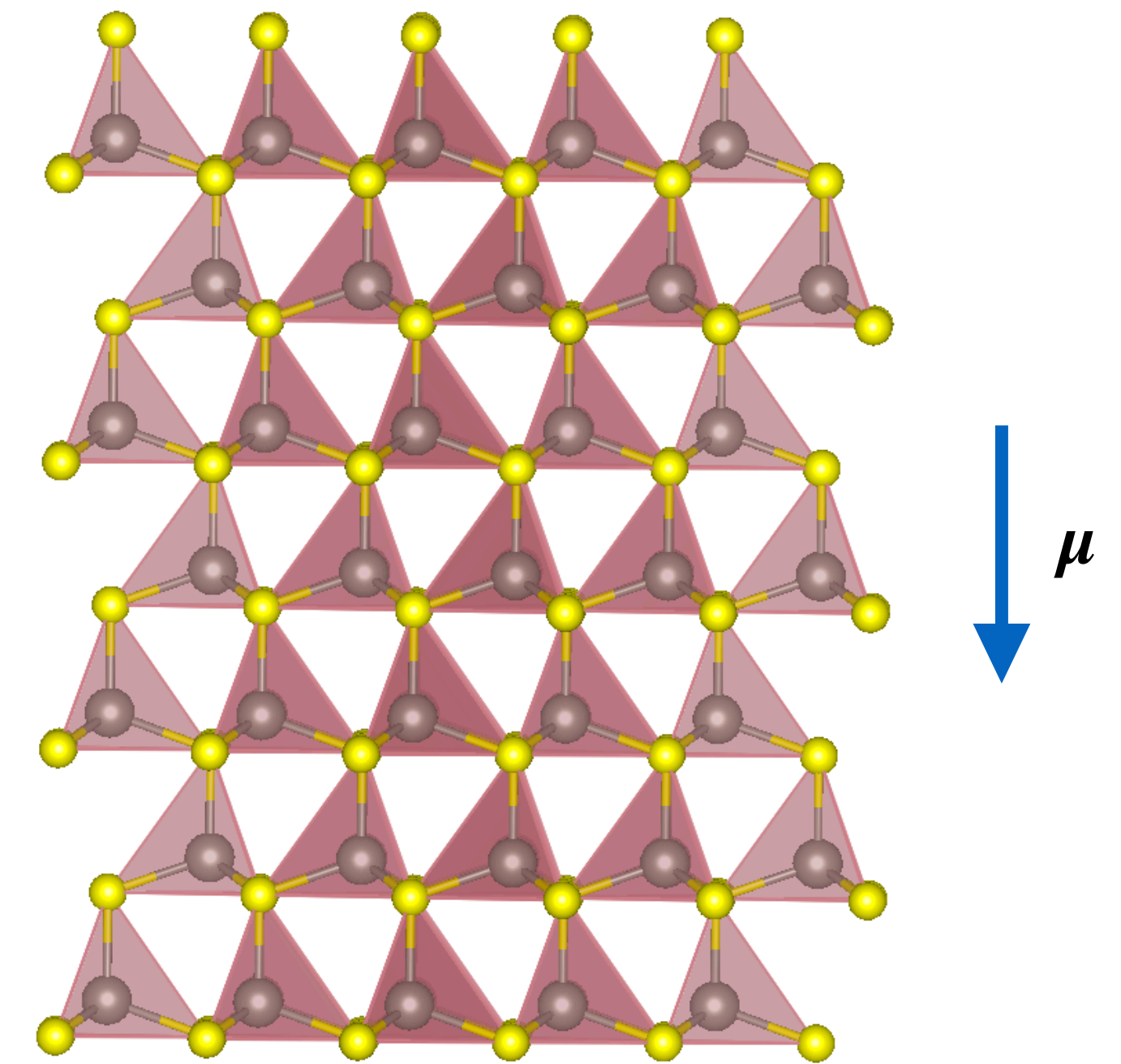
**noncentrosymmetric
crystal**

non-polar



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polar

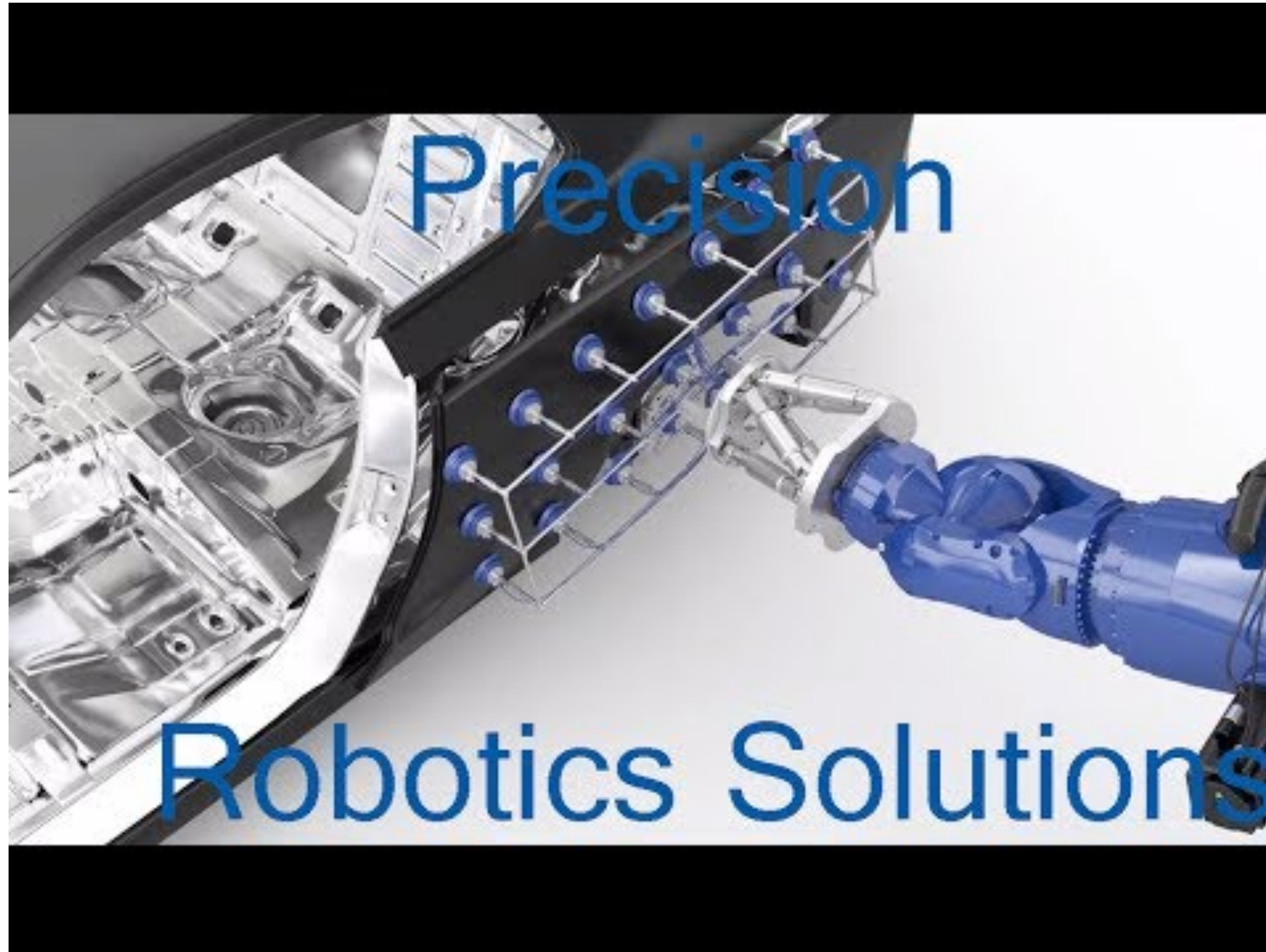


pyroelectricity

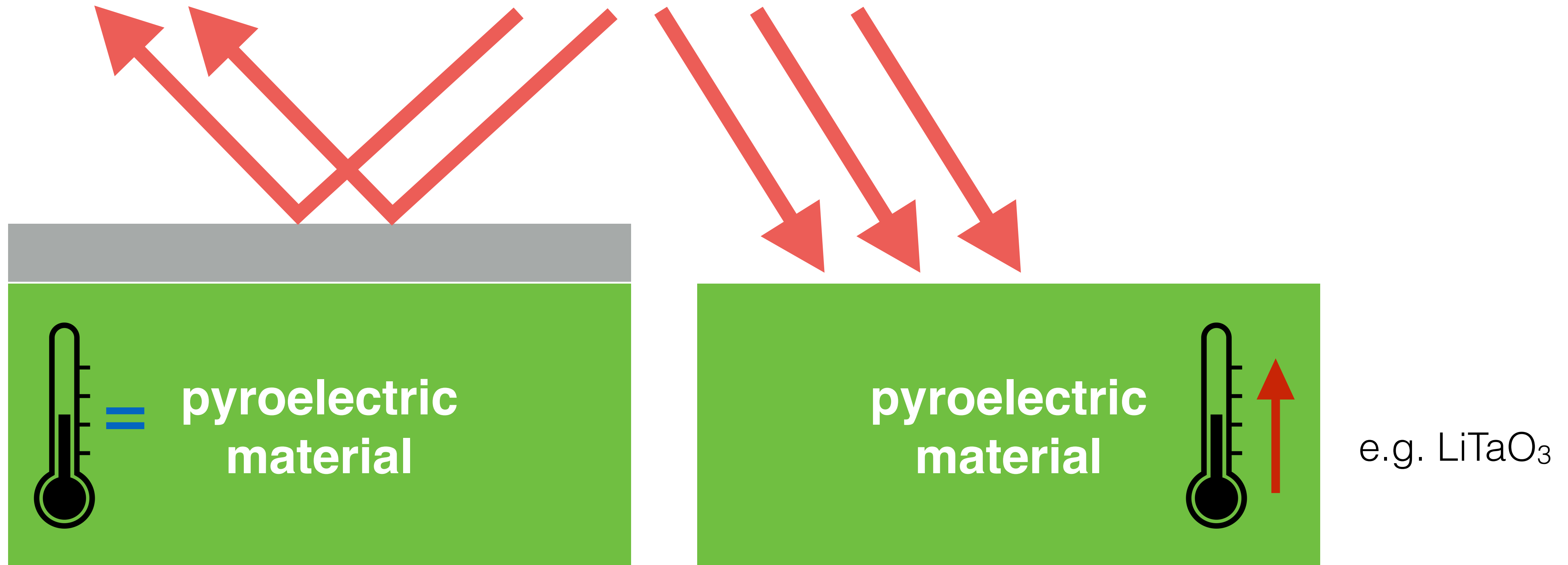
Applications of piezoelectricity: energy harvesting



Applications of piezoelectricity: hexapods

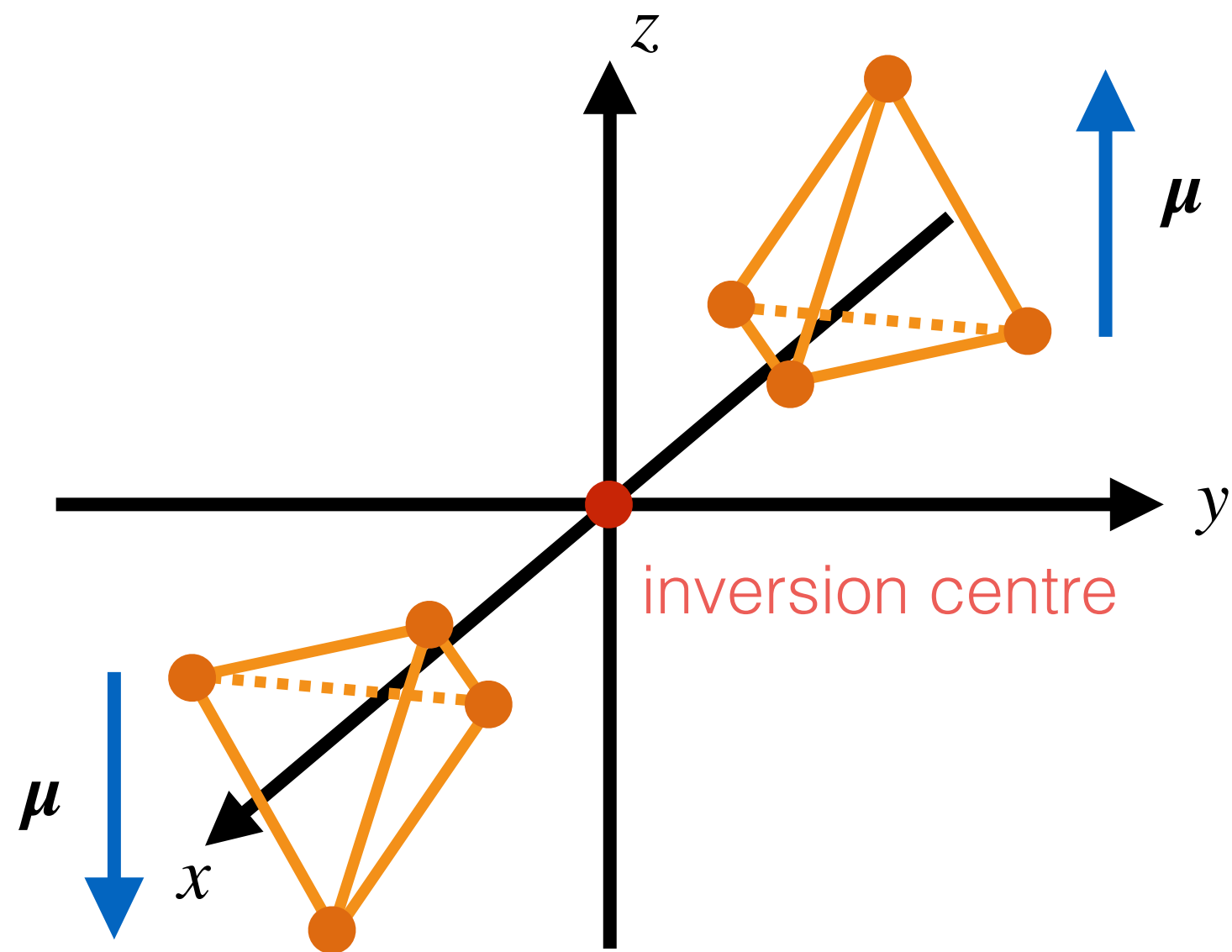


Applications of pyroelectricity: infrared detector



centrosymmetric crystal

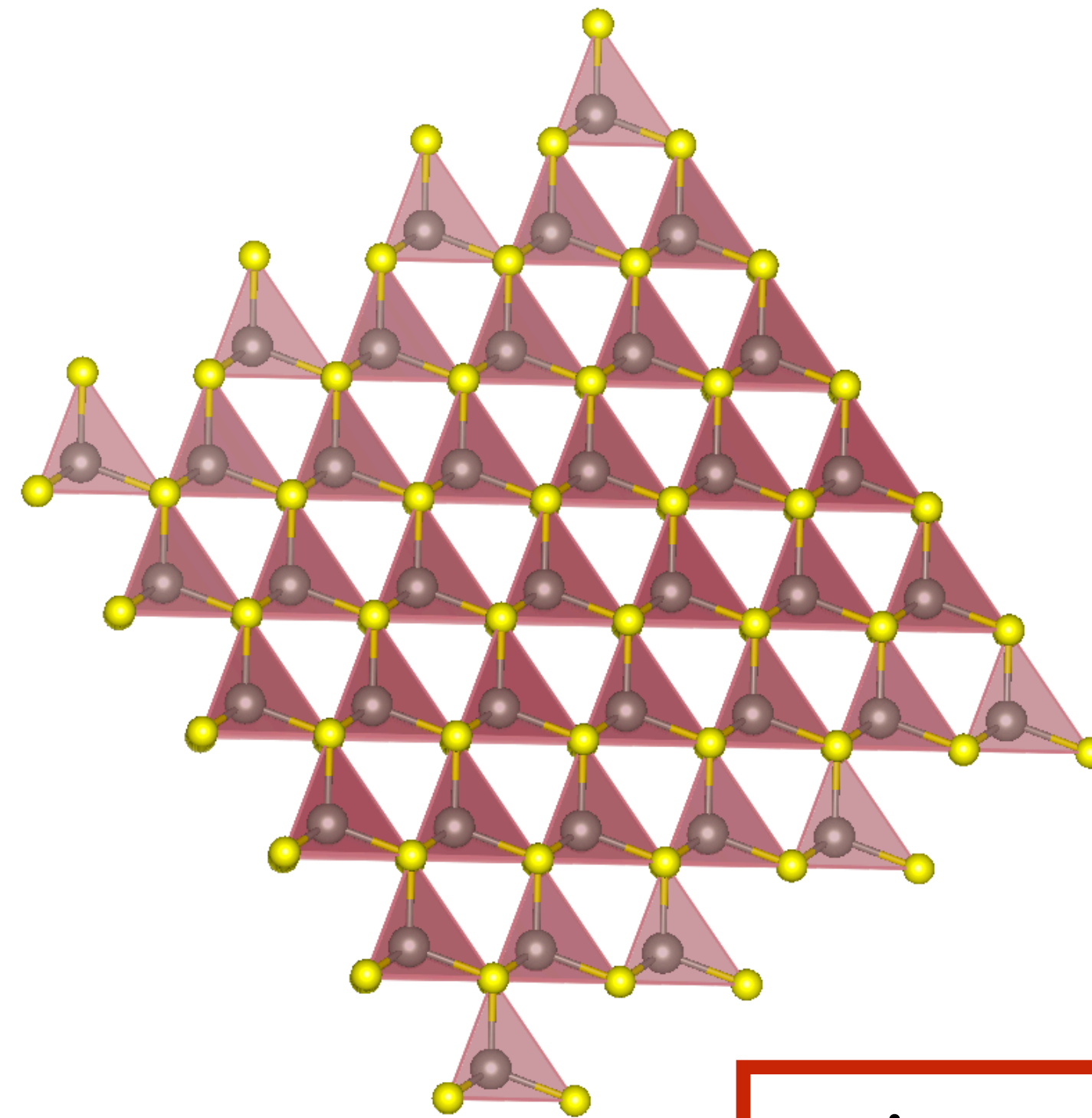
non-polar



no piezoelectricity

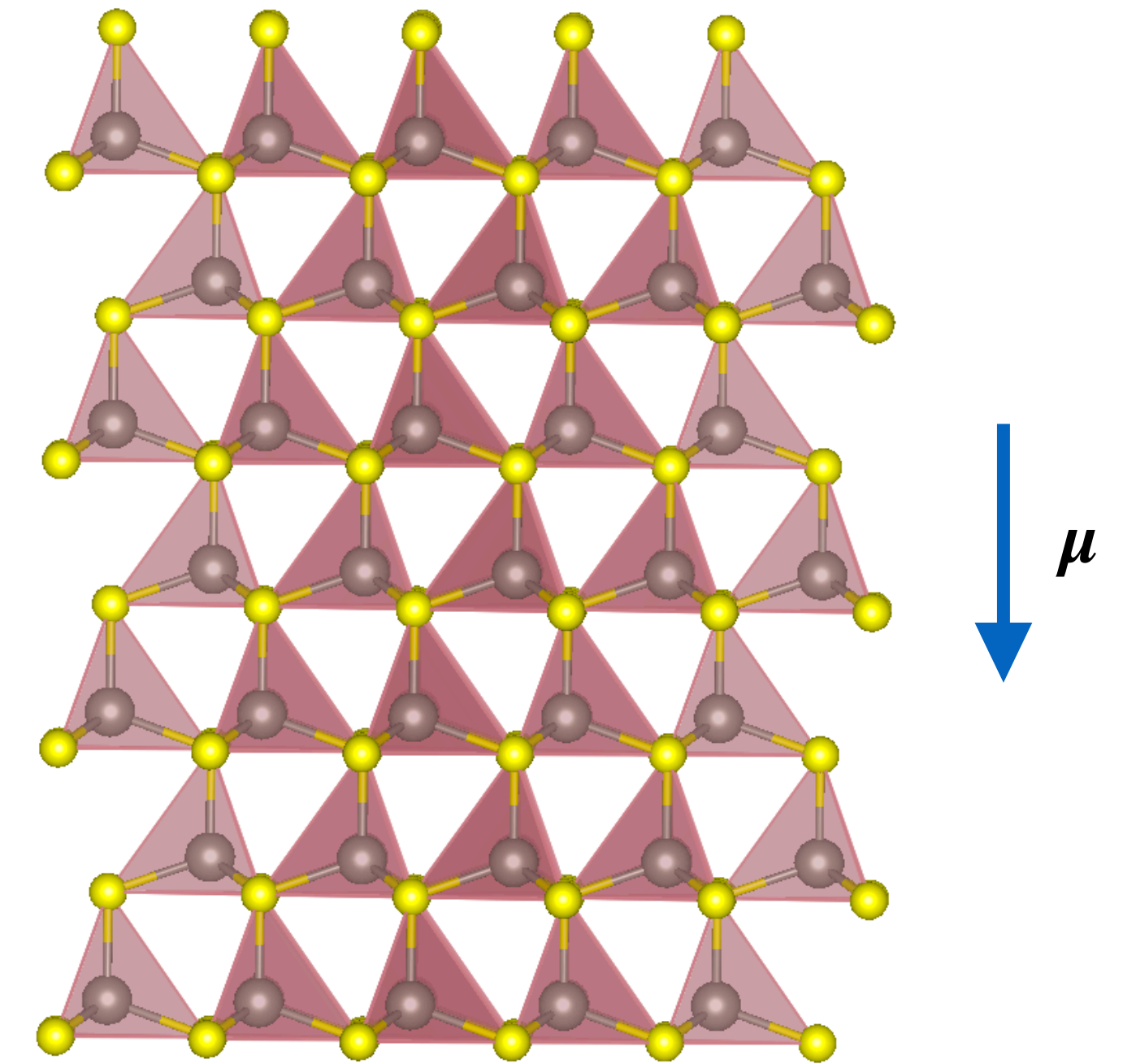
noncentrosymmetric crystal

non-polar



piezoelectricity*

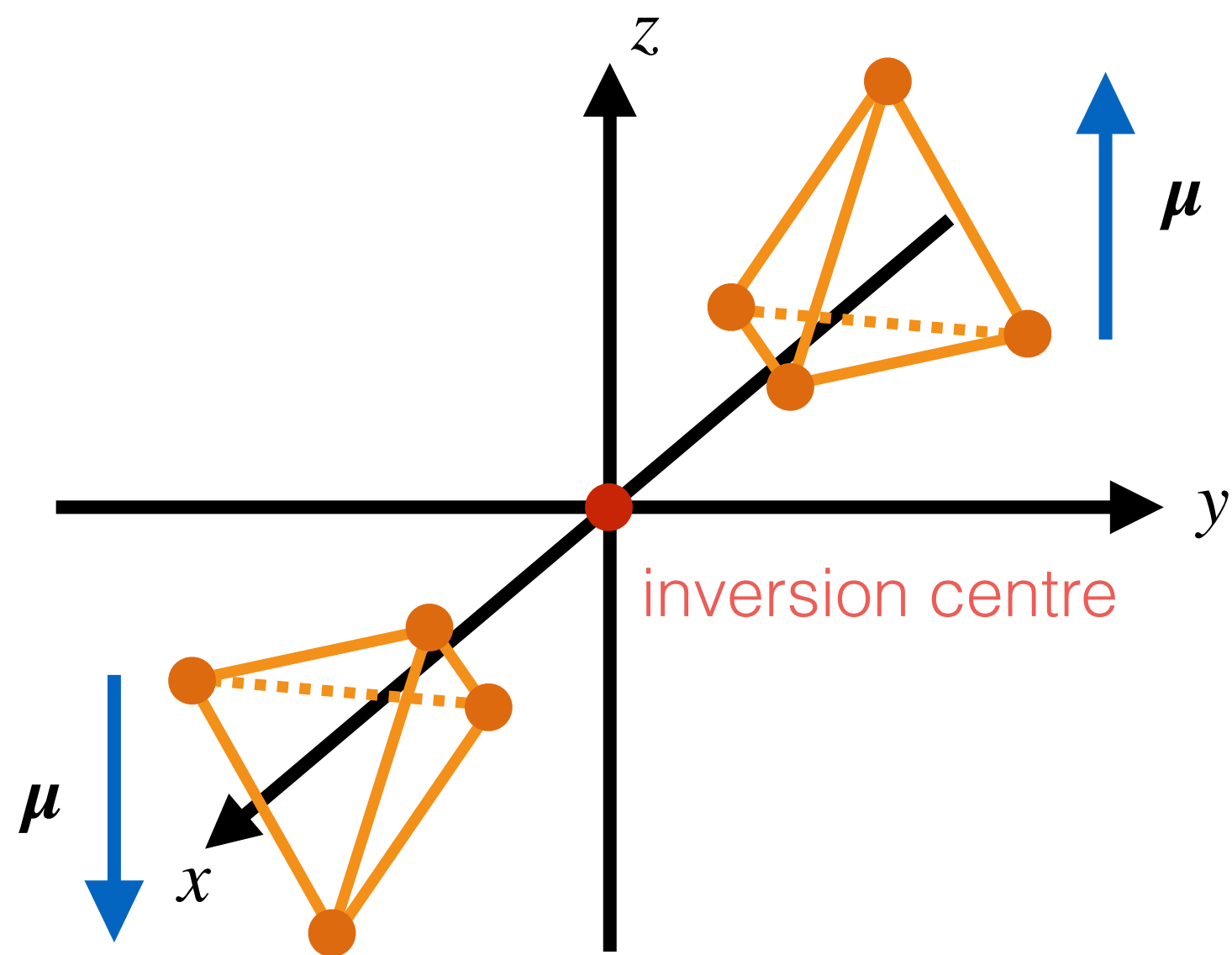
polar



* Cubic crystal class 432 exception

**centrosymmetric
crystal**

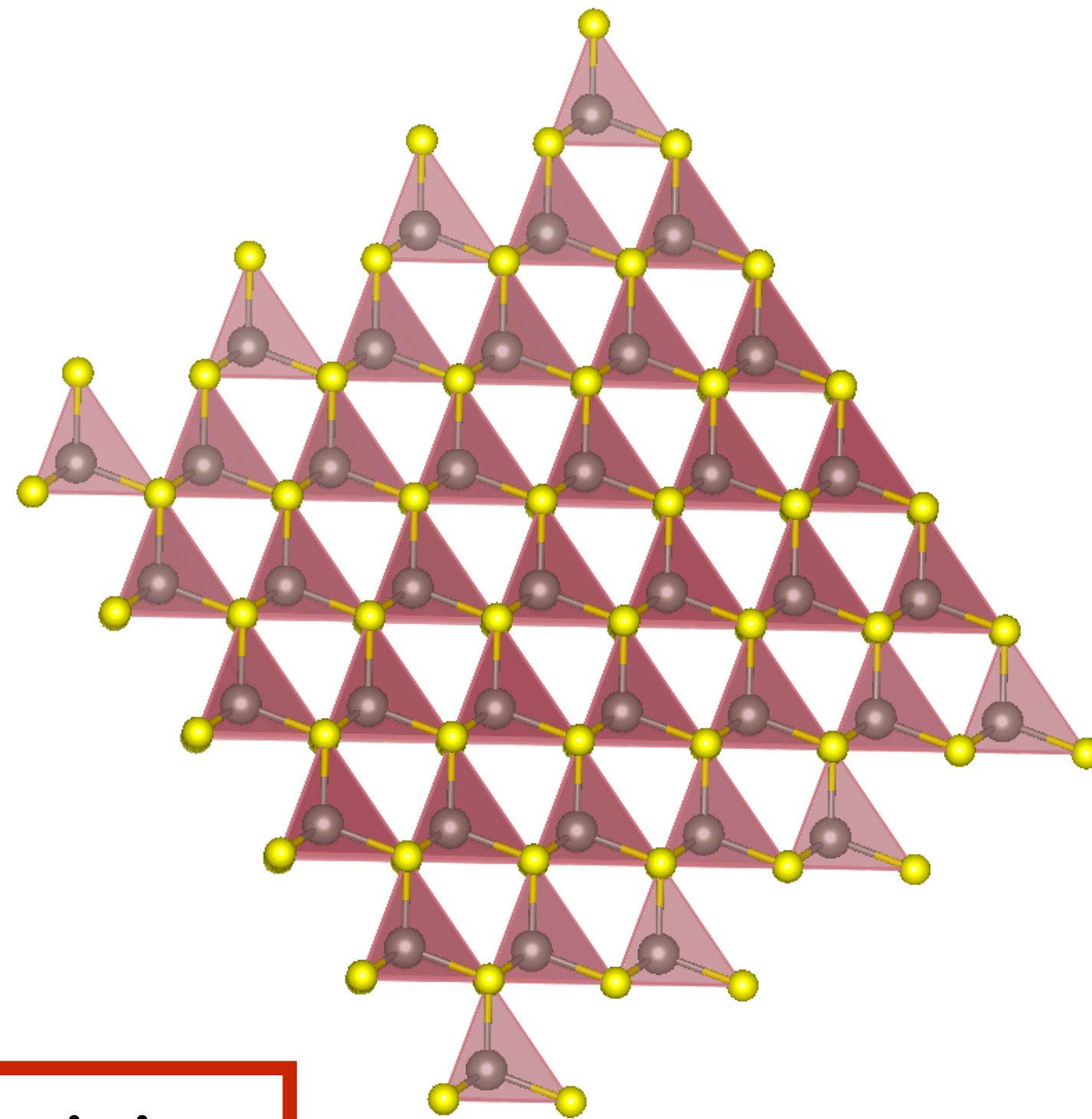
non-polar



no pyroelectricity

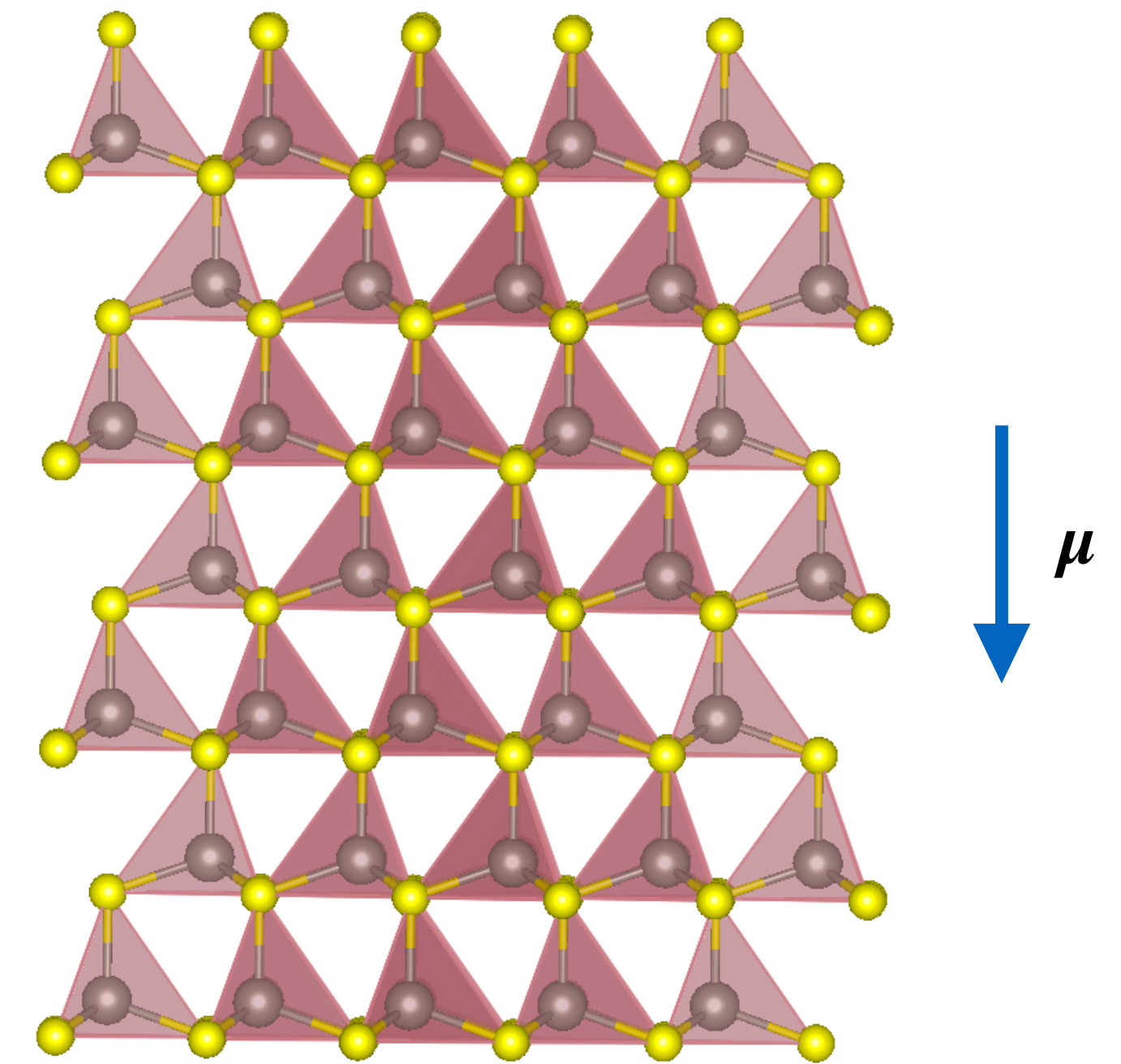
**noncentrosymmetric
crystal**

non-polar



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polar



pyroelectricity