Macroscopic polarization and related properties (BerryPI)

Oleg Rubel

Thunder Bay Regional Research Institute

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How did it start?

[Wien] Piezoelectric properties

The Mail Archive

Oleg Rubel | Thu, 14 Apr 2011 10:17:15 -0400

Dear Wien2k users and developers,

I am curious whether it is possible to extract piezoelectric properties (e.g., derivative of polarization with respect to strain) using Wien2k? It seems that there is no such a functionality documented in the UG, but maybe there some indirect ways. Ideally, it would be great to reproduce results of Saghi-Szabo et al. [PRL 80, 4321 (1998)] obtained using Berry's phase approach.

Thank you in advance
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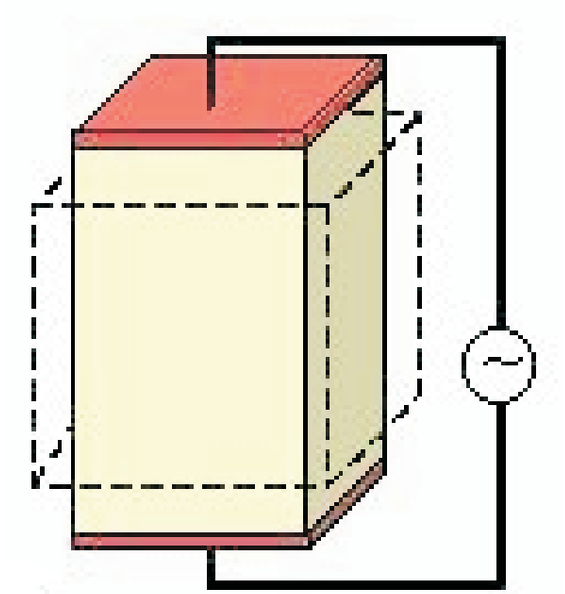
https://github.com/spichardo/BerryPI

Outline

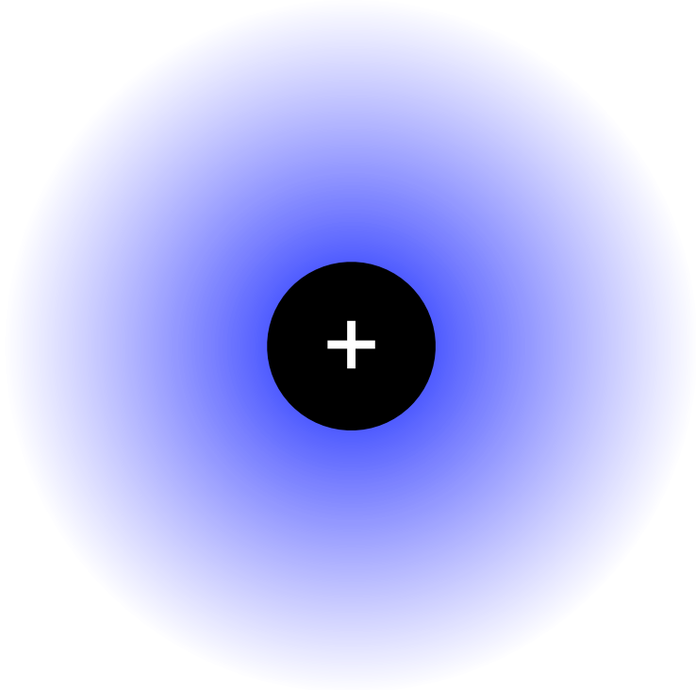
- Modern theory of polarization (Berry phase)
- `BerryPI` structure and execution
- Tutorials

Material properties related to polarization

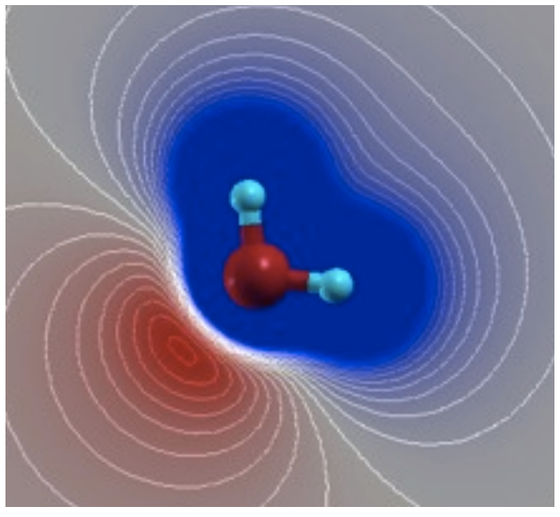
Piezoelectricity



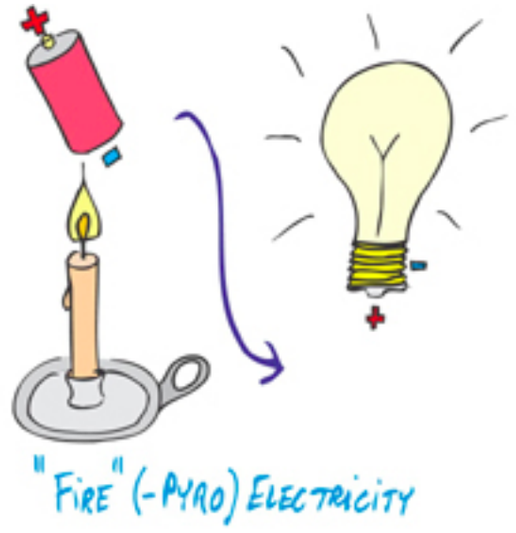
Dielectric screening



Effective charge



Pyroelectricity



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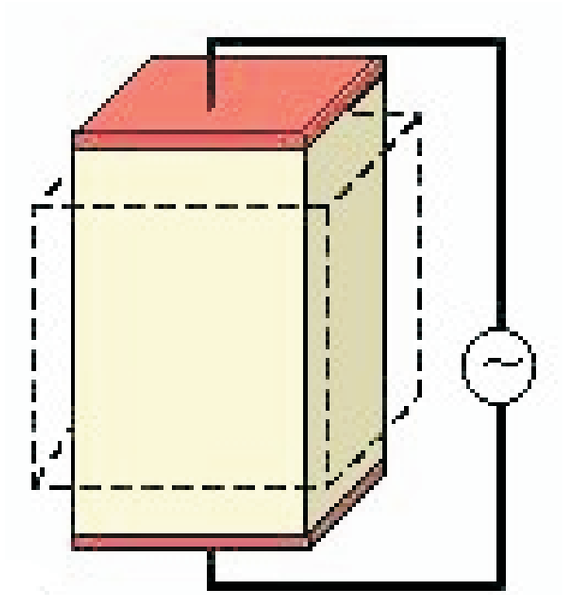

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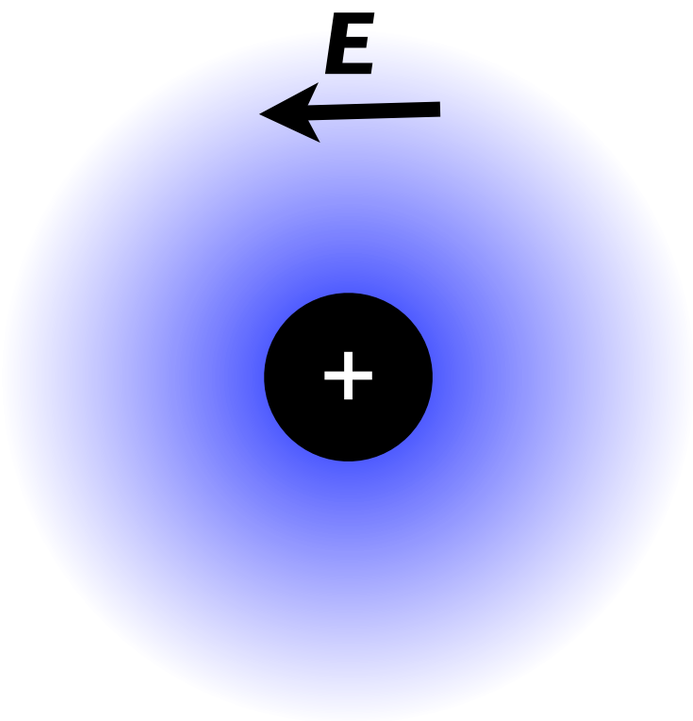

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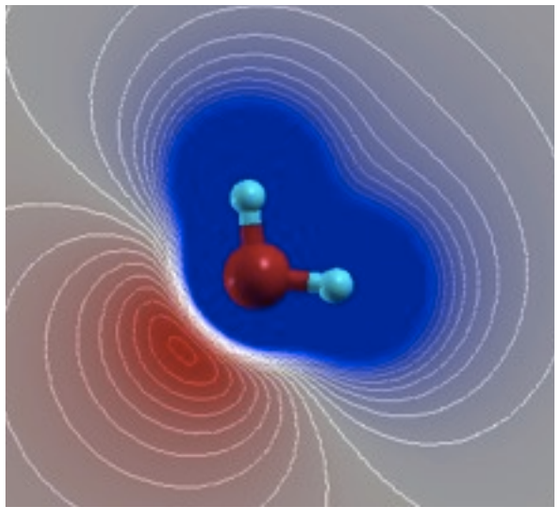

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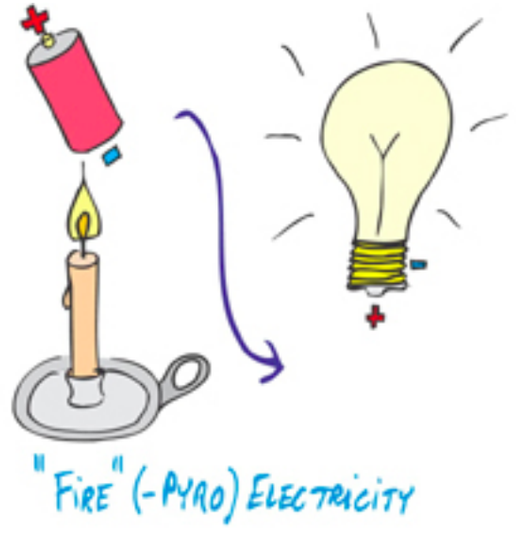

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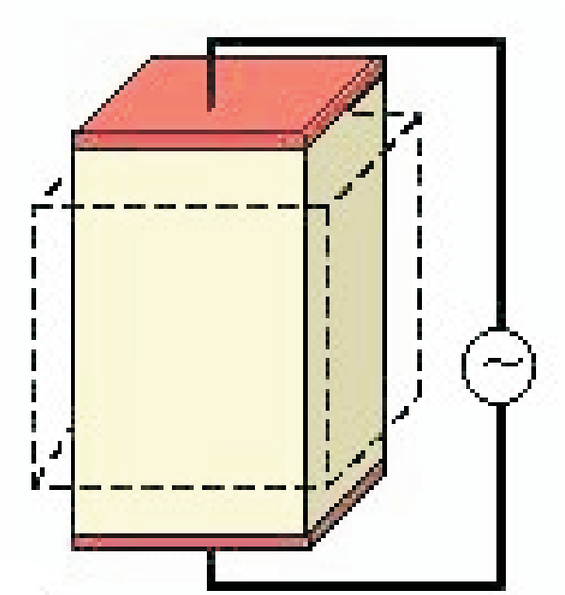

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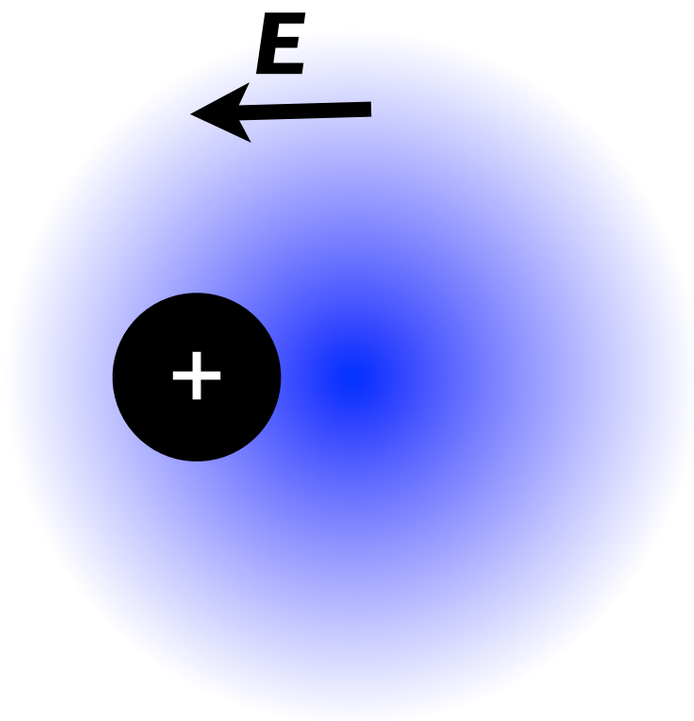

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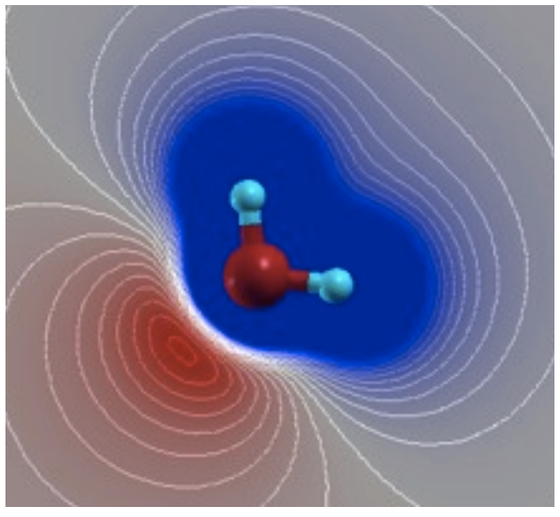

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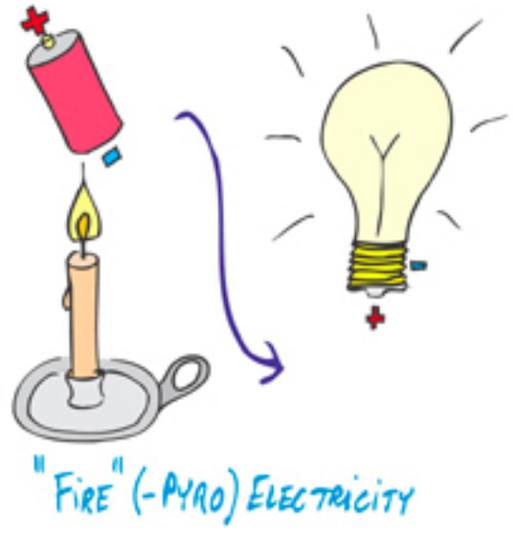

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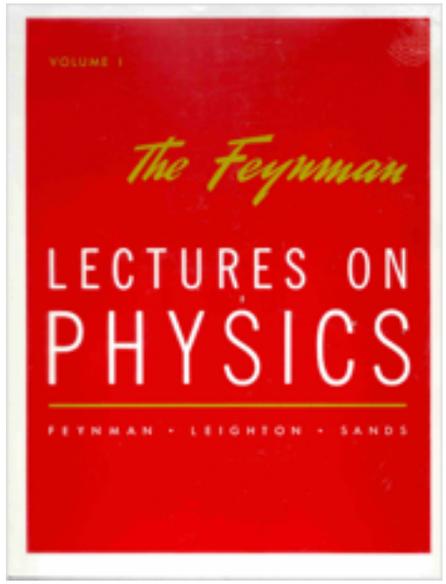

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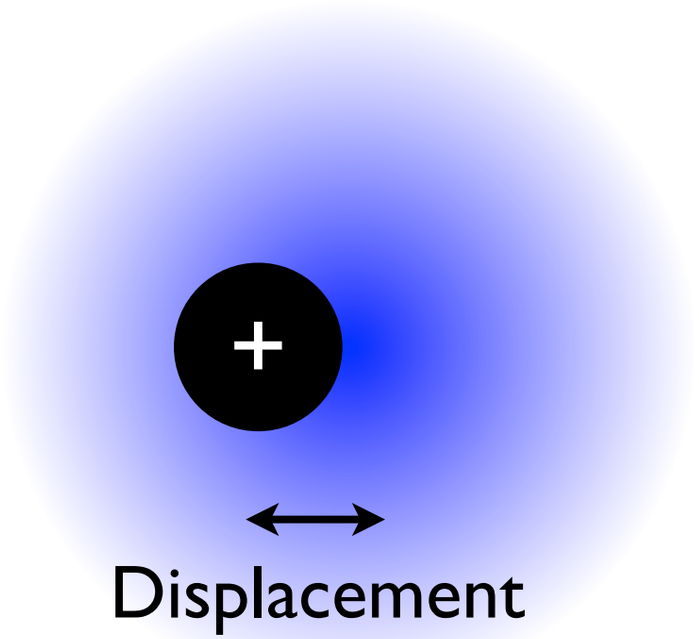

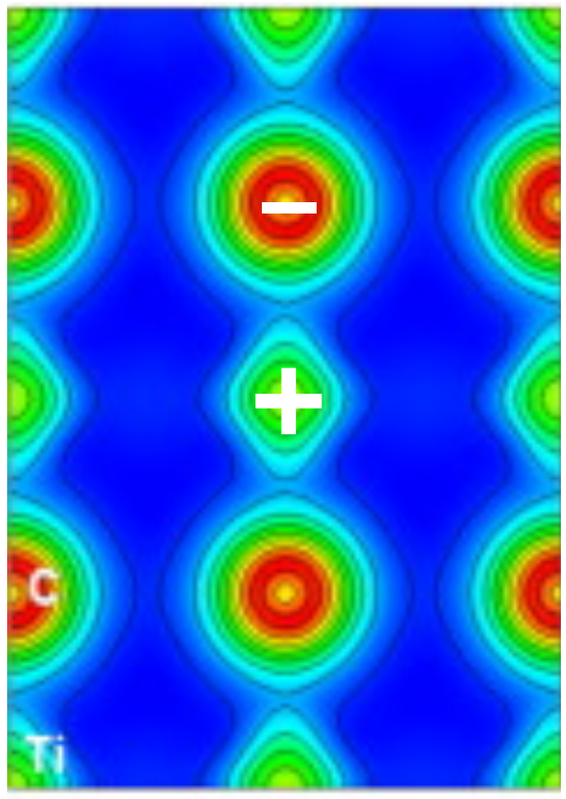

Polarization for periodic solids is undefined

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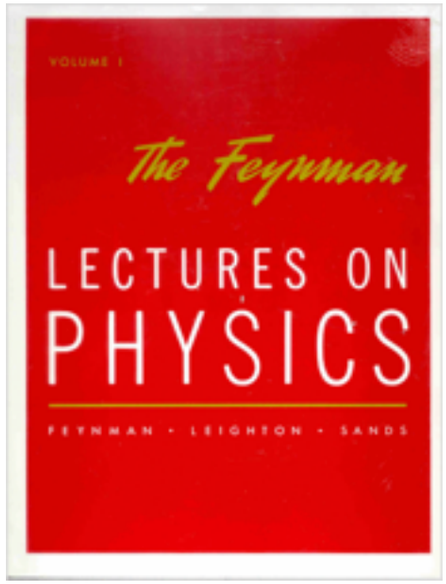

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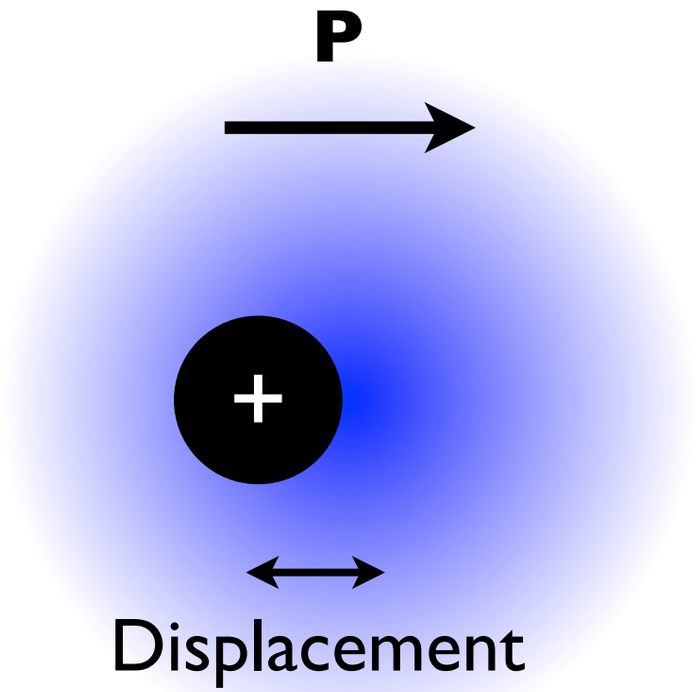

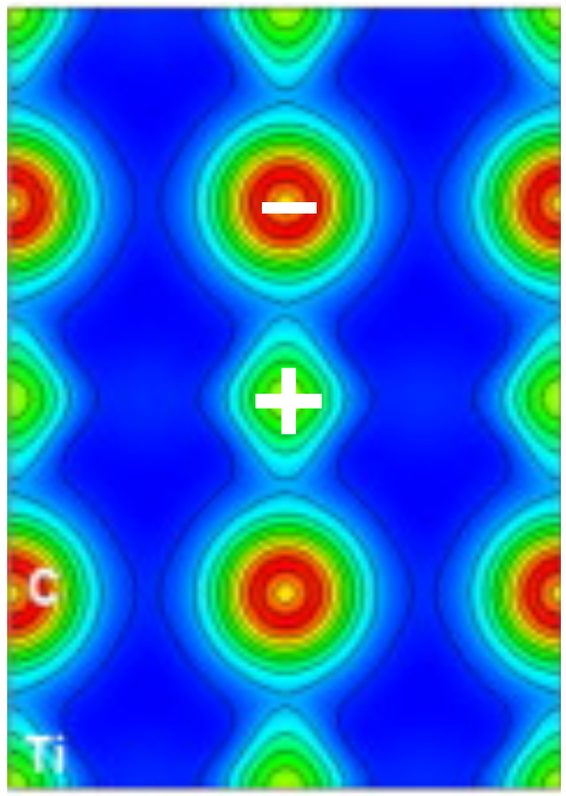

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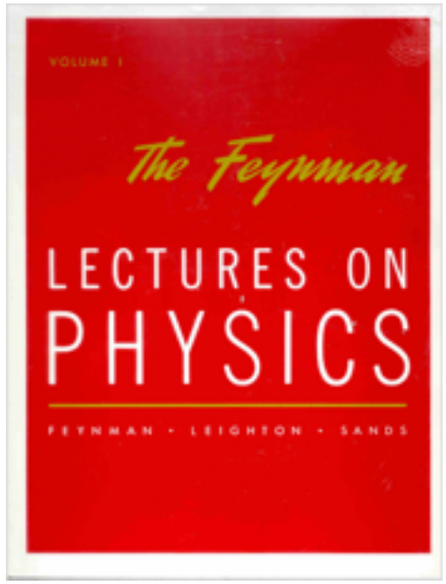

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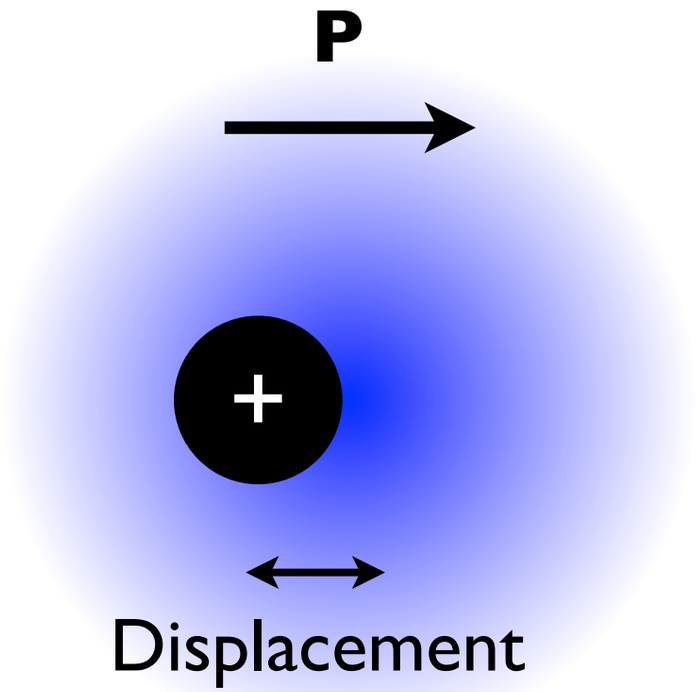

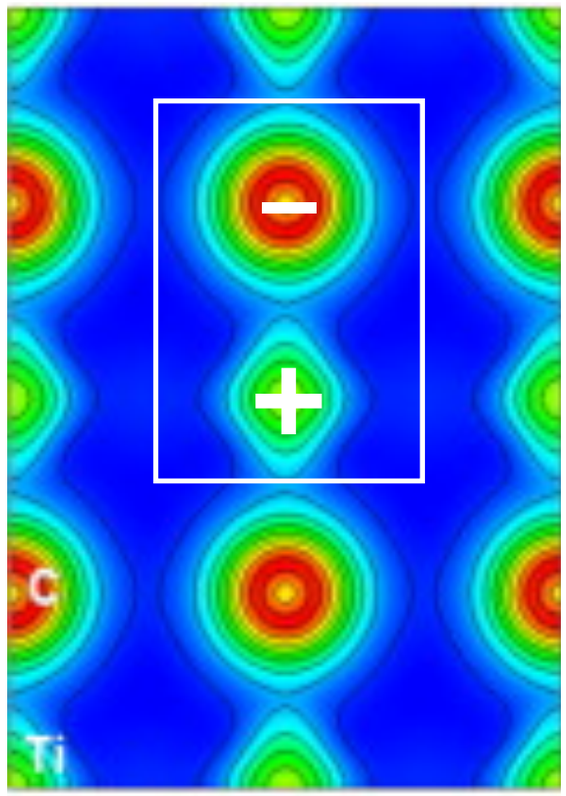

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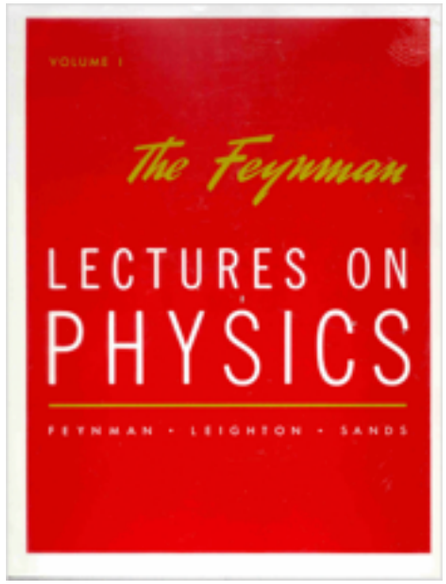

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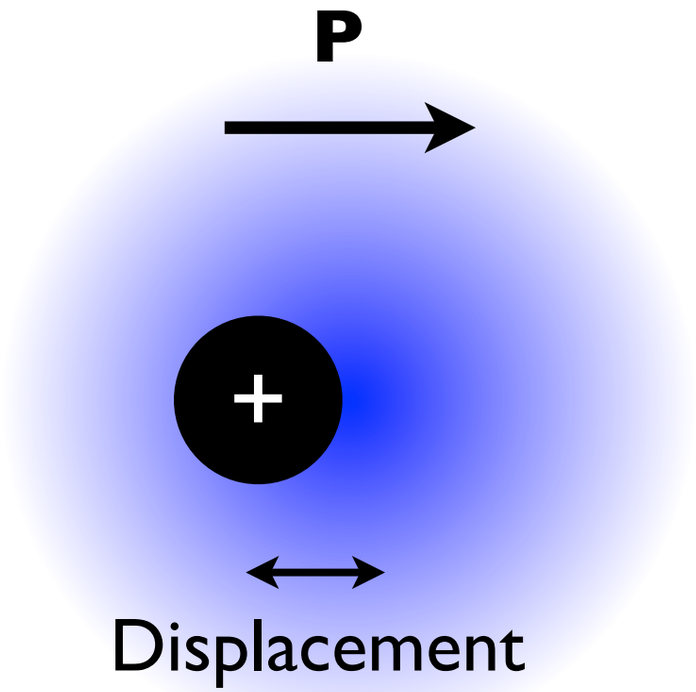

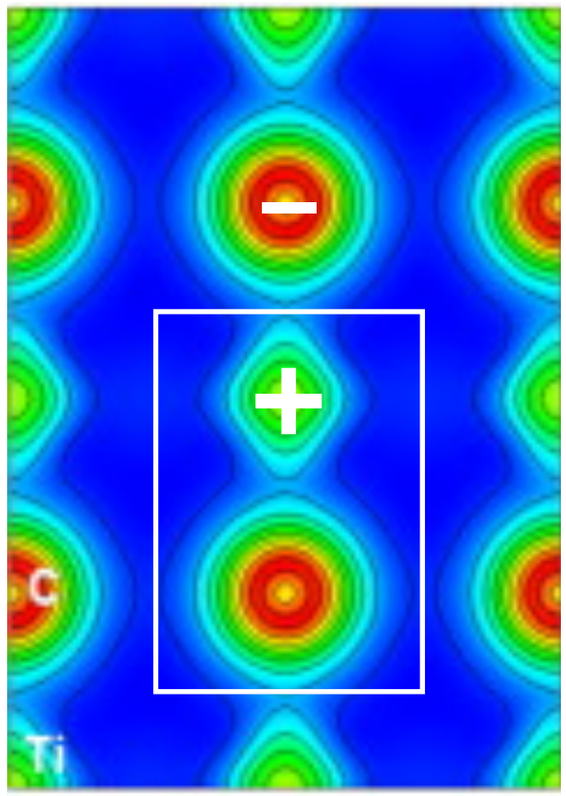

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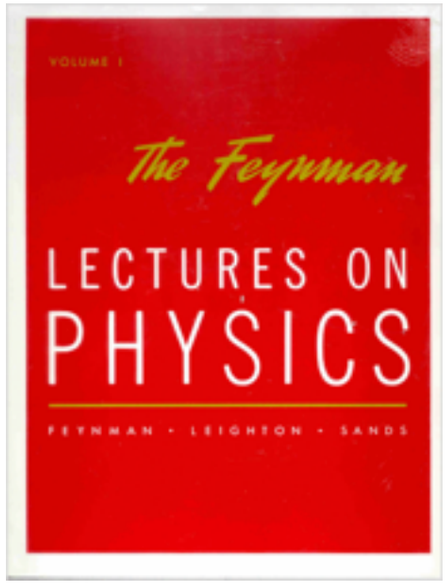

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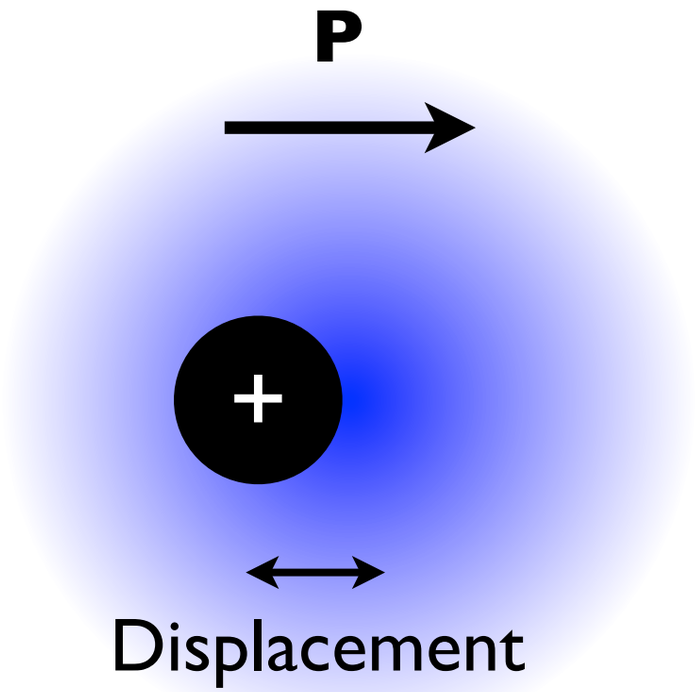

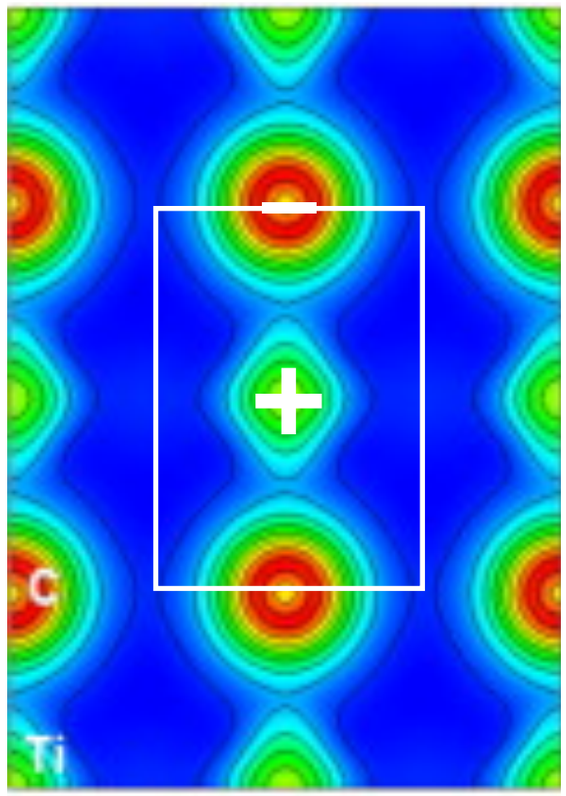

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Modern theory of polarization

Pioneered by *King-Smith*, *David Vanderbilt* and *Raffaele Resta*

All measurable physical quantities are related to the **change** in polarization!

$$\Delta\mathbf{P} = \mathbf{P}^{(0)} - \mathbf{P}^{(1)}$$

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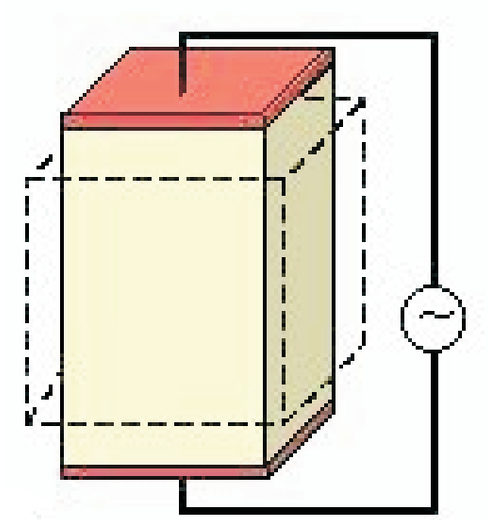

$$\frac{\Delta \mathbf{P}}{\Delta \text{strain}}$$

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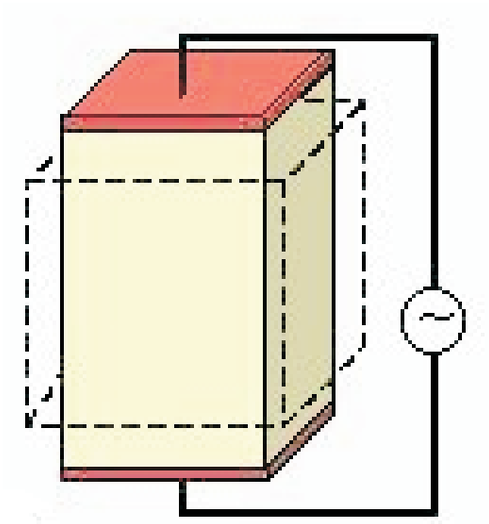

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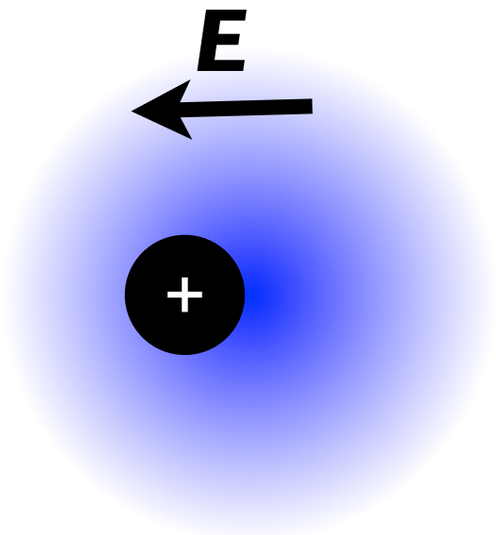

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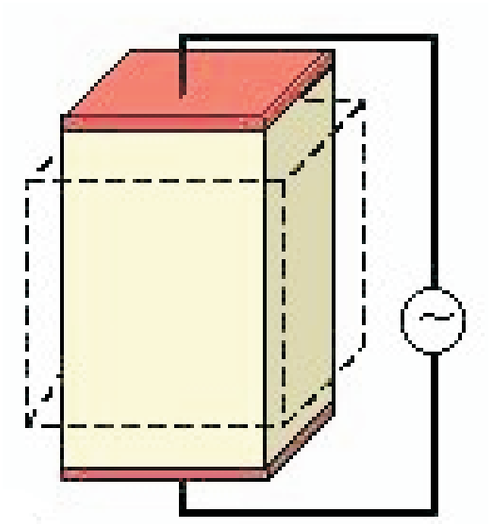

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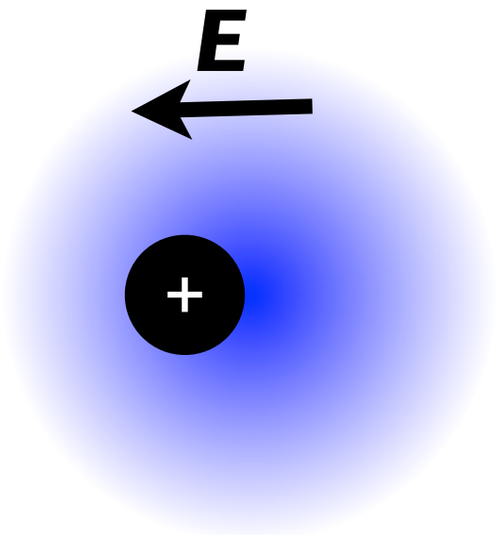

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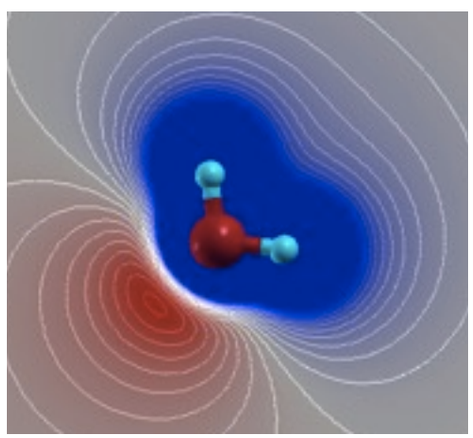

$$\frac{\Delta \mathbf{P}}{\text{displacement}}$$

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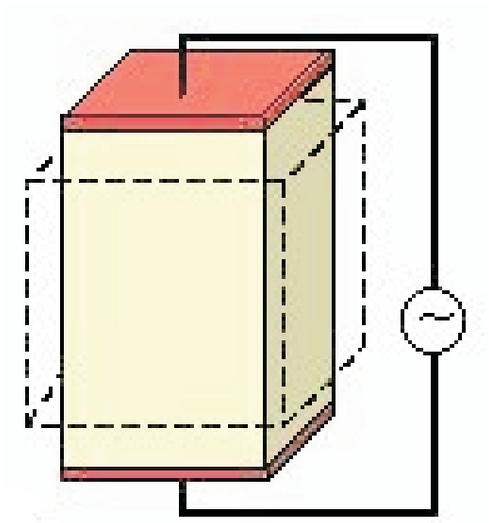

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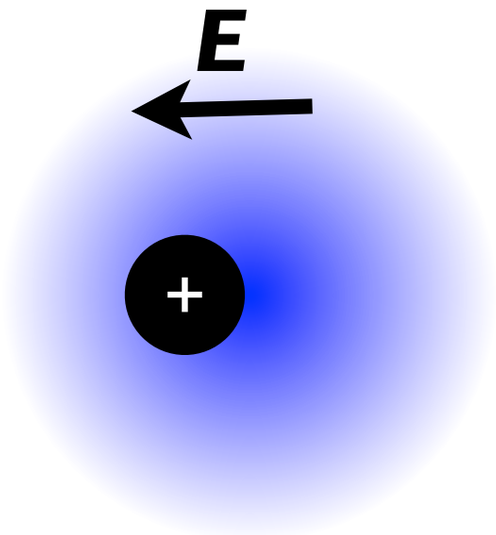

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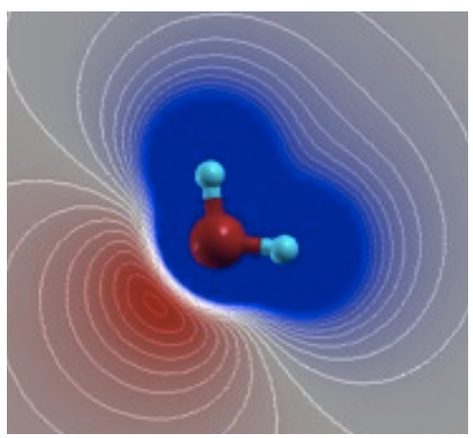


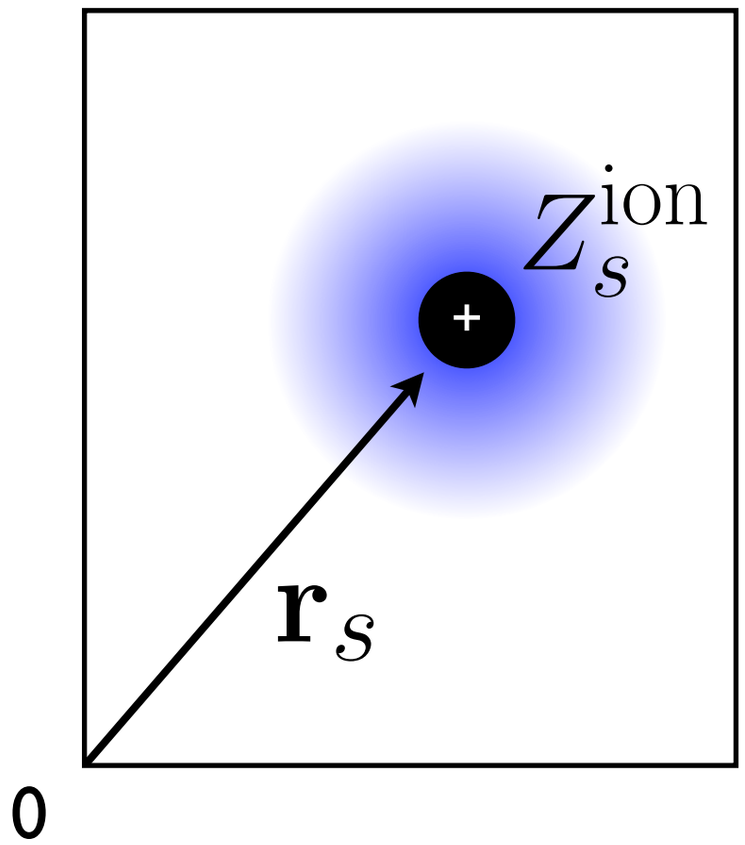
$$\frac{\Delta \mathbf{P}}{\text{displacement}}$$

$$\frac{\Delta \mathbf{P}}{\Delta T}$$

Polarization as a transient current

$$\Delta\mathbf{P} = \mathbf{P}^{(1)} - \mathbf{P}^{(0)} = \Omega^{-1} \int dt \int_{\text{cell}} d\mathbf{r}\, \mathbf{j}(\mathbf{r}, t)$$

transient current density



$$\mathbf{P} = \mathbf{P}_{\text{ion}} + \mathbf{P}_{\text{el}}$$

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In Wien2k Z_s^{ion} is the core charge

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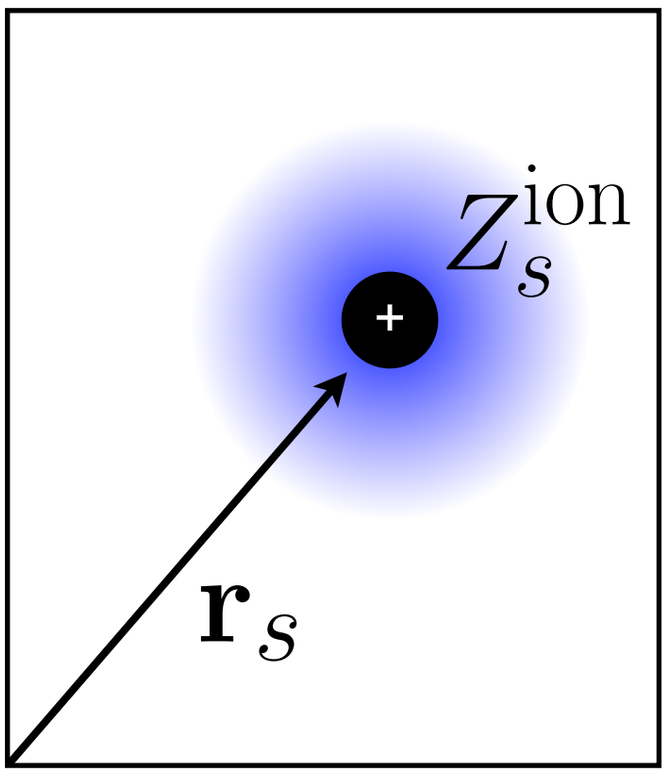

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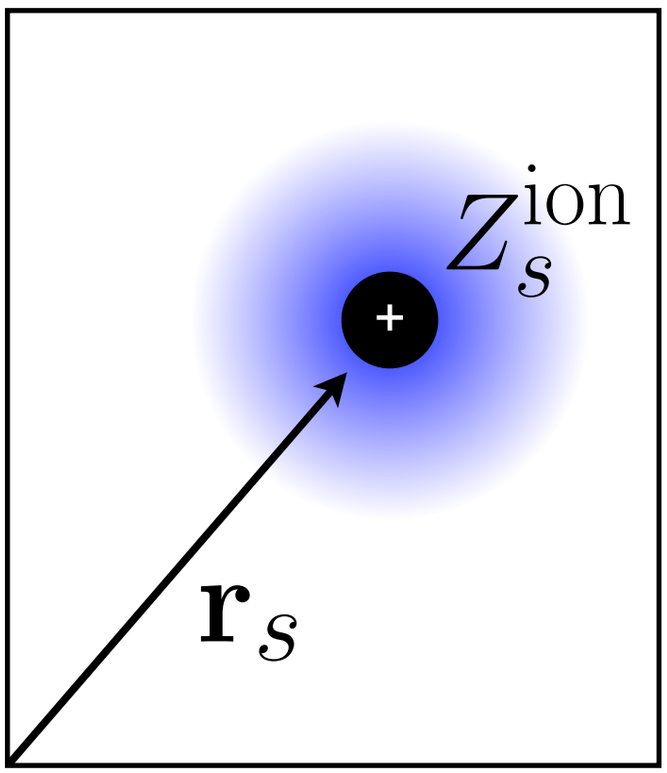

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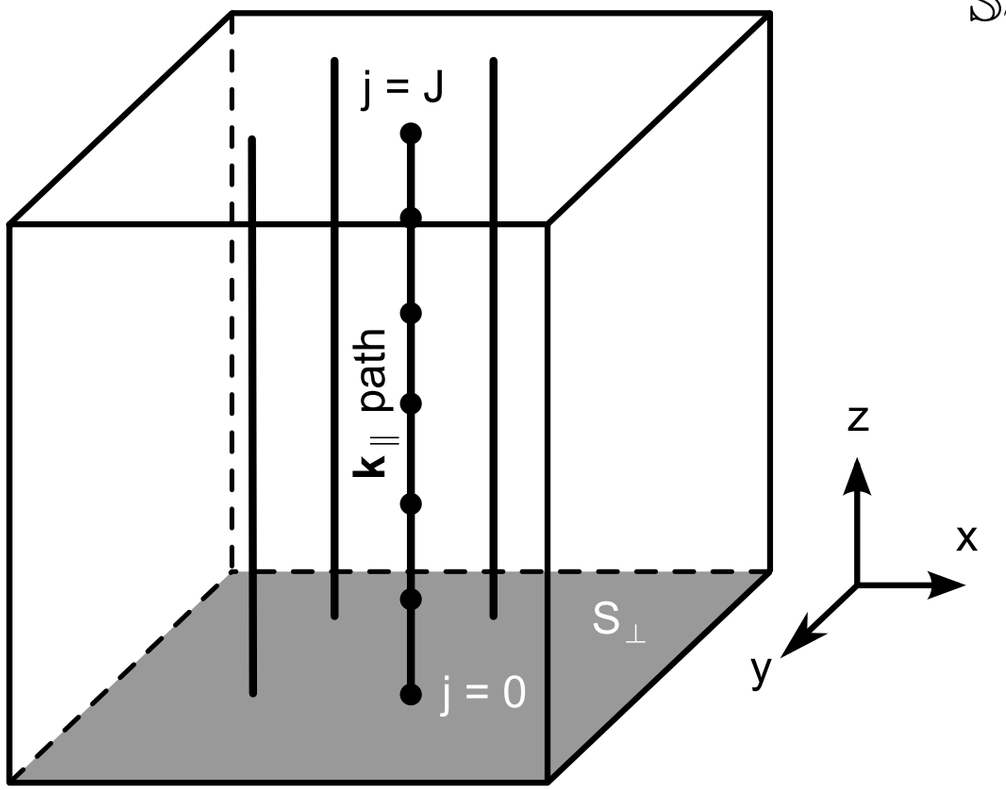
Berry phase

$$\mathrm{d}\varphi_n = -i\langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}}|u_{n\mathbf{k}}\rangle \cdot \mathrm{d}\mathbf{k} = -i\,\ln\langle u_{n\mathbf{k}}|u_{n(\mathbf{k}+\mathrm{d}\mathbf{k})}\rangle$$



$$\mathbb{S}_{mn}(\mathbf{k}_j, \mathbf{k}_{j+1}) = \langle u_{m\mathbf{k}_j}|u_{n\mathbf{k}_{j+1}}\rangle$$ WIEN2WANNIER

$$\varphi(\mathbf{k}_\parallel) = 2\,\mathrm{Im}\left[\ln\prod_{j=0}^{J-1}\det\mathbb{S}_{M\times M}(\mathbf{k}_j, \mathbf{k}_{j+1})\right]$$

$$\varphi_{\mathrm{el},\alpha} = S_\perp^{-1}\int_{S_\perp}\mathrm{d}S_\perp\;\varphi(\mathbf{k}_\parallel)$$

$$P_\alpha = \frac{e(\varphi_{\mathrm{el},\alpha} + \varphi_{\mathrm{ion},\alpha})}{2\pi\Omega}\,R_\alpha$$

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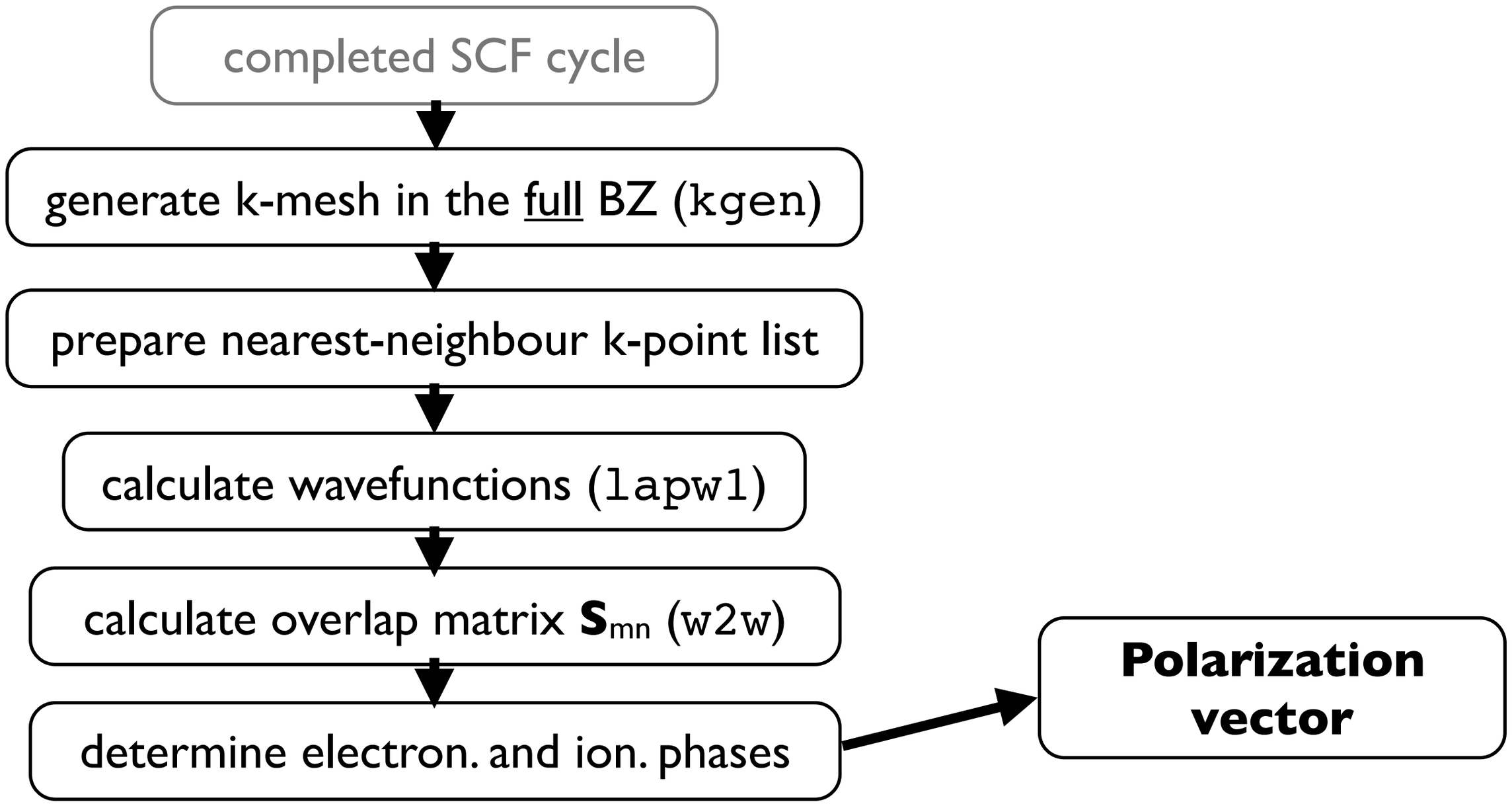
BerryPI

Need `wien2k`, `wien2wannier`, `python` 2.7.x and `numpy`

```
[command line]$ berrypi -p($pwd) -k6:6:6
```



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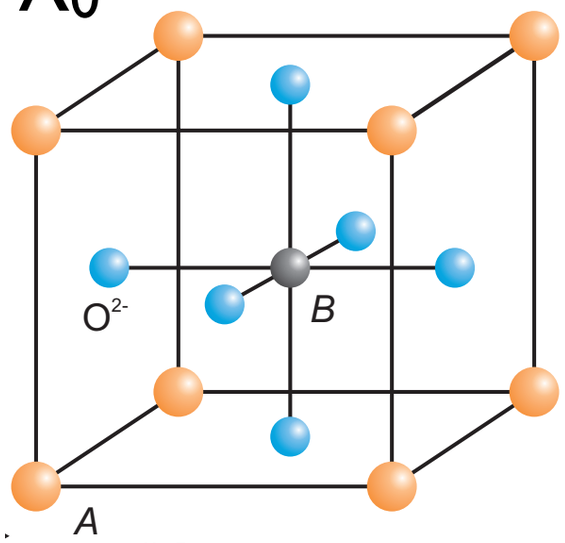
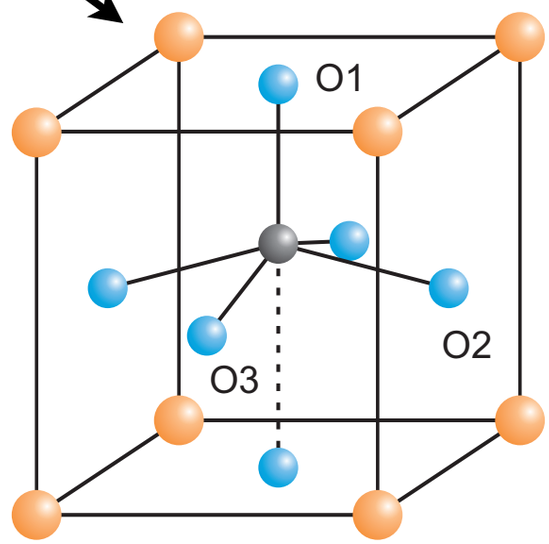
Two cases: λ_0 and λ_1

$$\Delta \mathbf{P} = \mathbf{P}^{(0)} - \mathbf{P}^{(1)}$$

λ_0



λ_1



- structure file must preserve the symmetry
- begin with the lowest symmetry (λ_1) case
- copy case λ_1 to case λ_0
- edit structure file for case λ_0
- do not initialize calculation (`init_lapw`)
- update density (`x dstart`)
- run SCF cycle (`run_lapw`)
- run `BerryPI`

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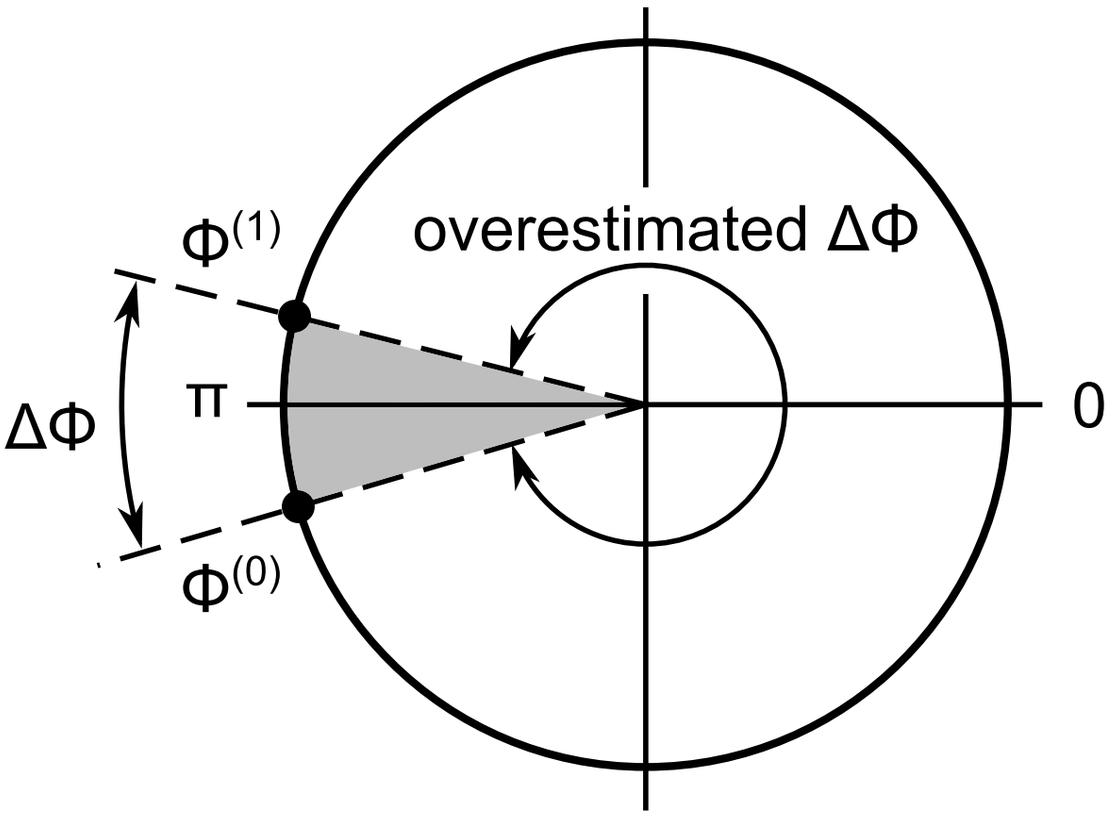
Uncertainties



$$P_\alpha = \frac{e(\varphi_{\mathrm{el},\alpha} + \varphi_{\mathrm{ion},\alpha})}{2\pi\Omega} R_\alpha$$

$$\Delta\mathbf{P} = \mathbf{P}^{(0)} - \mathbf{P}^{(1)} \pm \frac{e}{\Omega}\mathbf{R}$$

- cannot determine large polarization difference

Solution: $\lambda_1 \Rightarrow \lambda_{1/2} \Rightarrow \lambda_1$

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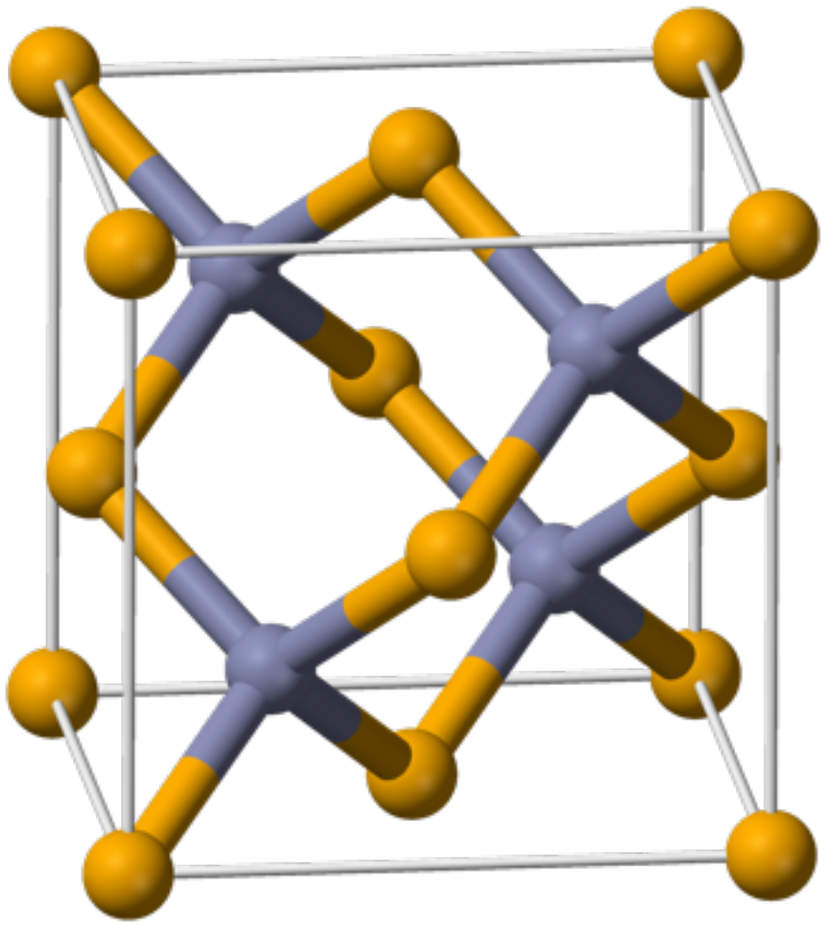
Current limitations



Non-orthogonal lattice vectors

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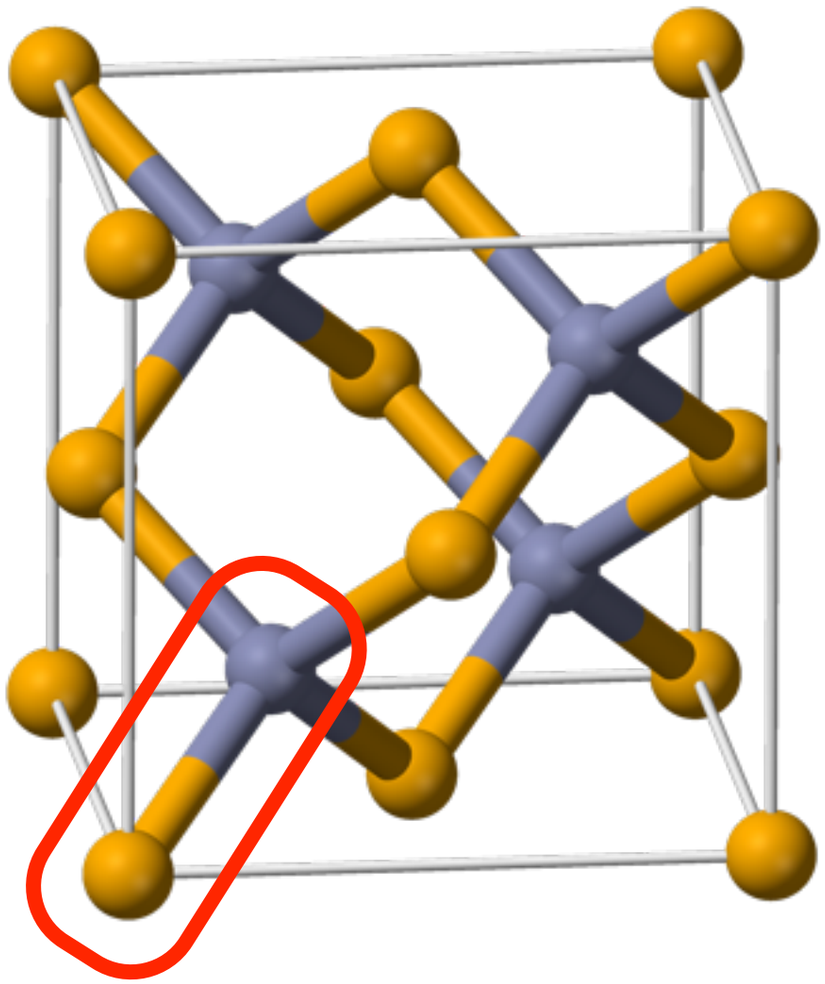
Current limitations



2-atom primitive basis

Non-orthogonal lattice vectors

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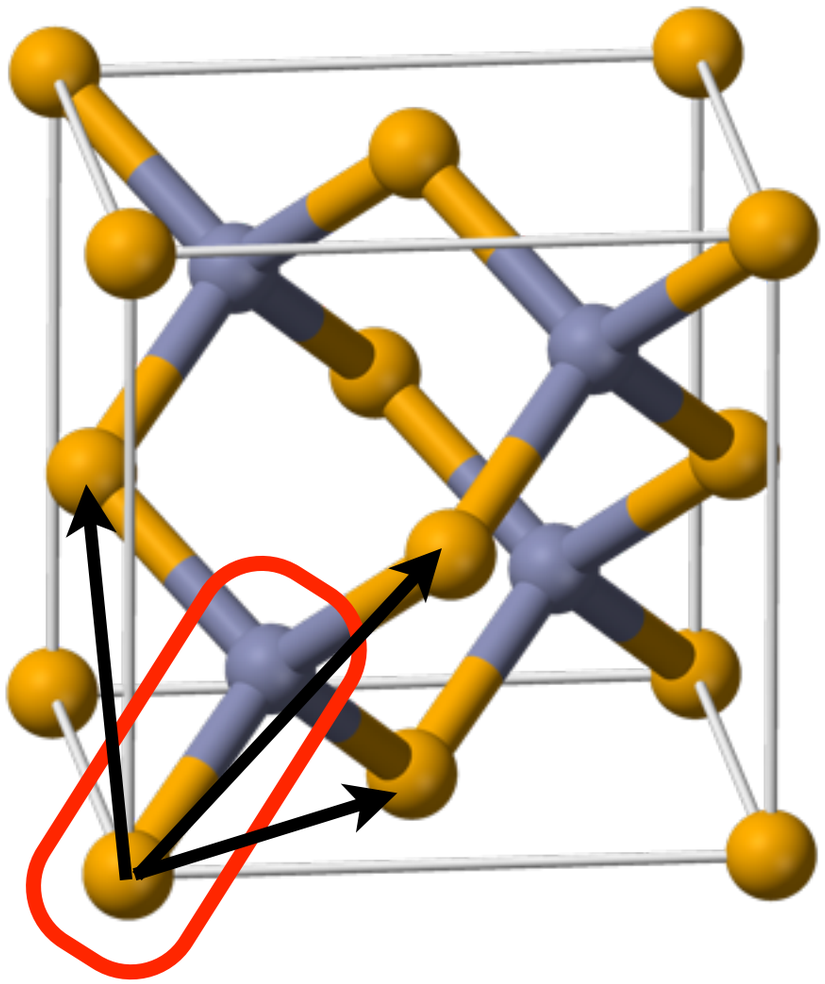
Current limitations



2-atom primitive basis

Non-orthogonal lattice vectors

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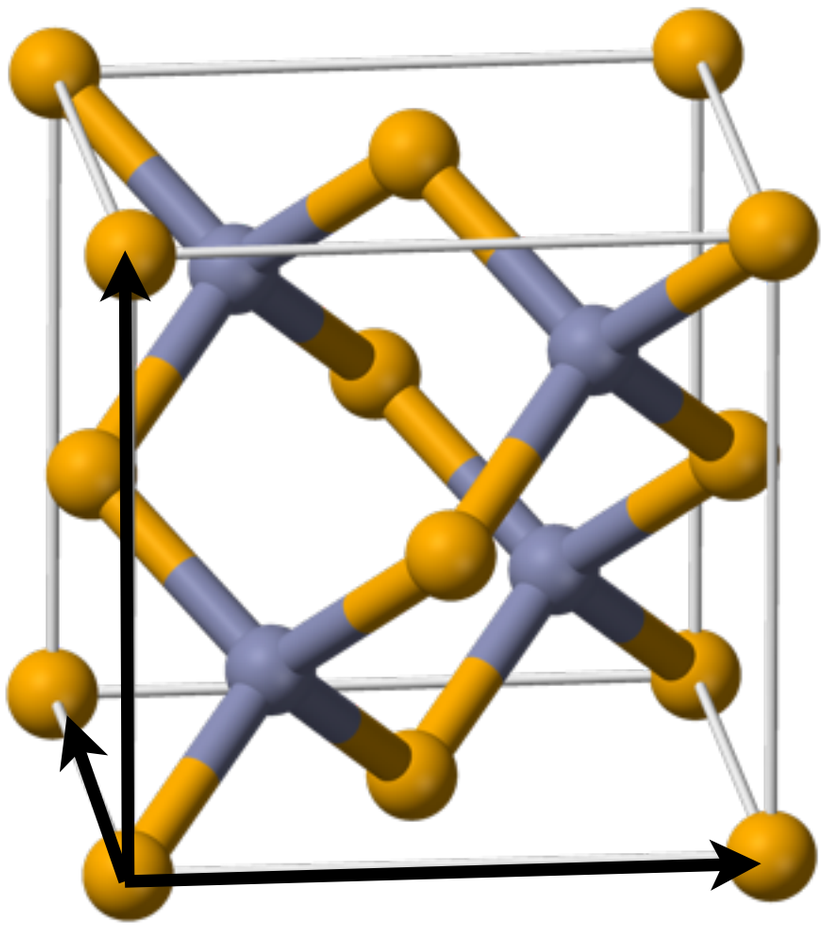
Current limitations



8-atom basis

Non-orthogonal lattice vectors

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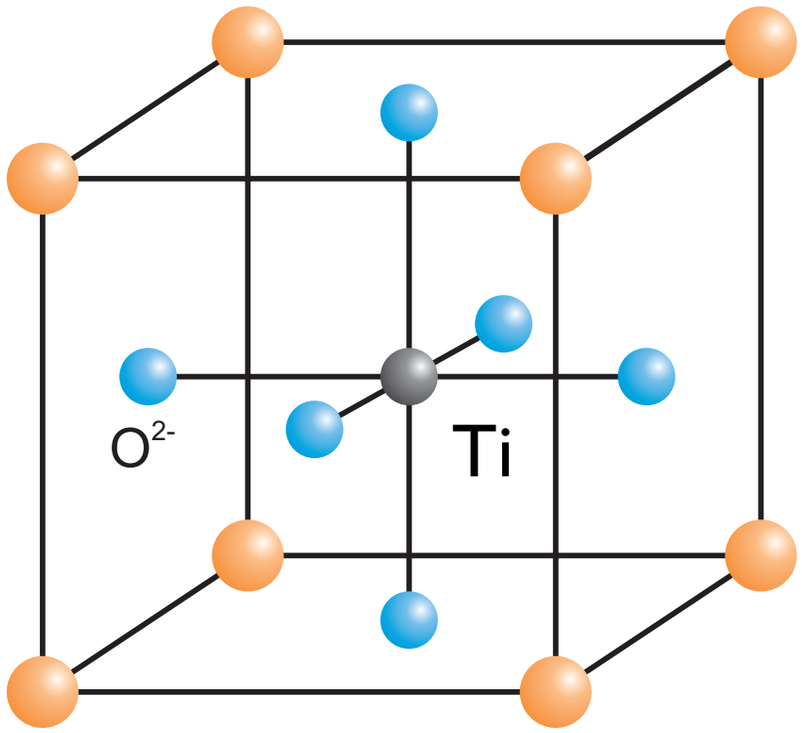
Tutorial 1: Spontaneous polarization

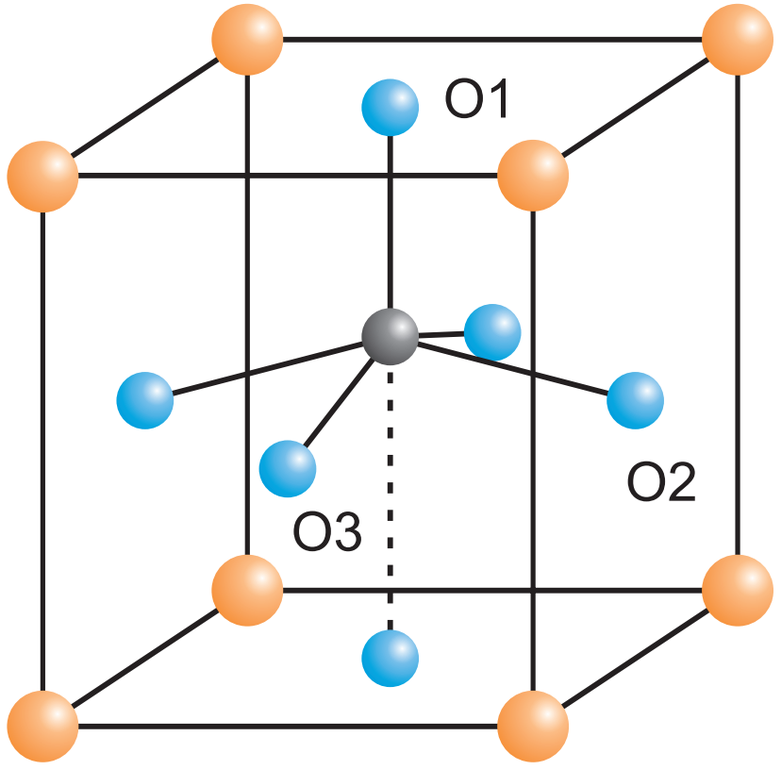
λ_0



Ba

centrosymmetric

λ_1

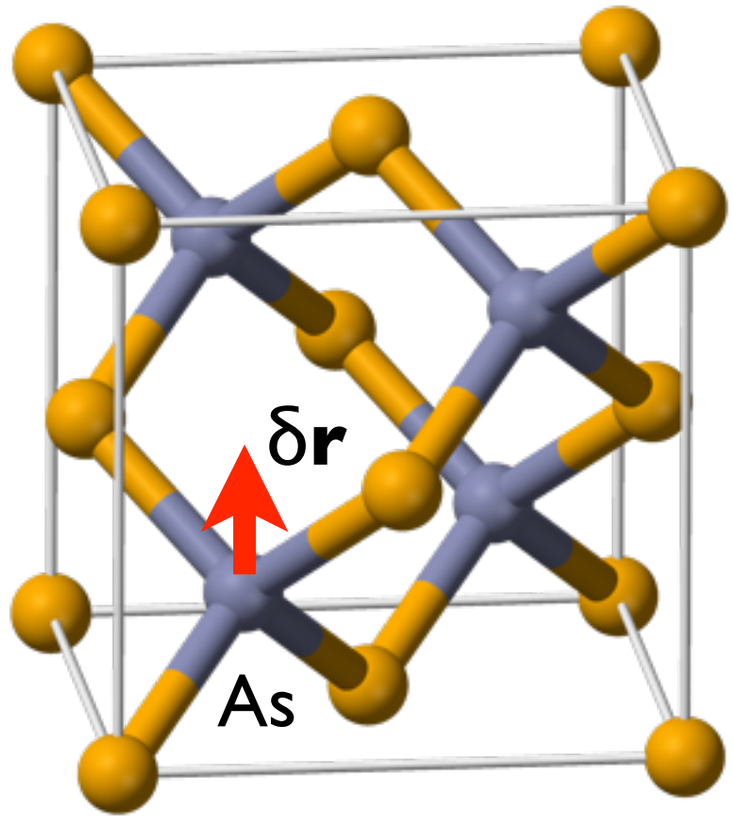


ferroelectric tetragonal

$$P_{\mathrm{S}} = P_{\mathrm{nc}} - P_{\mathrm{c}}$$

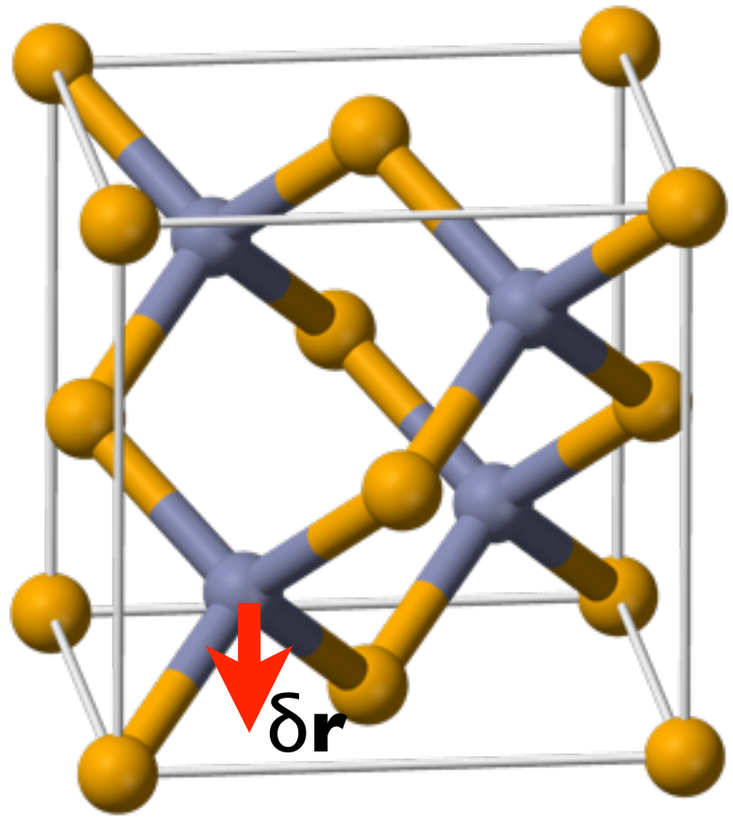
Tutorial 2: Born effective charge

λ_1



displacement +δ**r**

λ_2

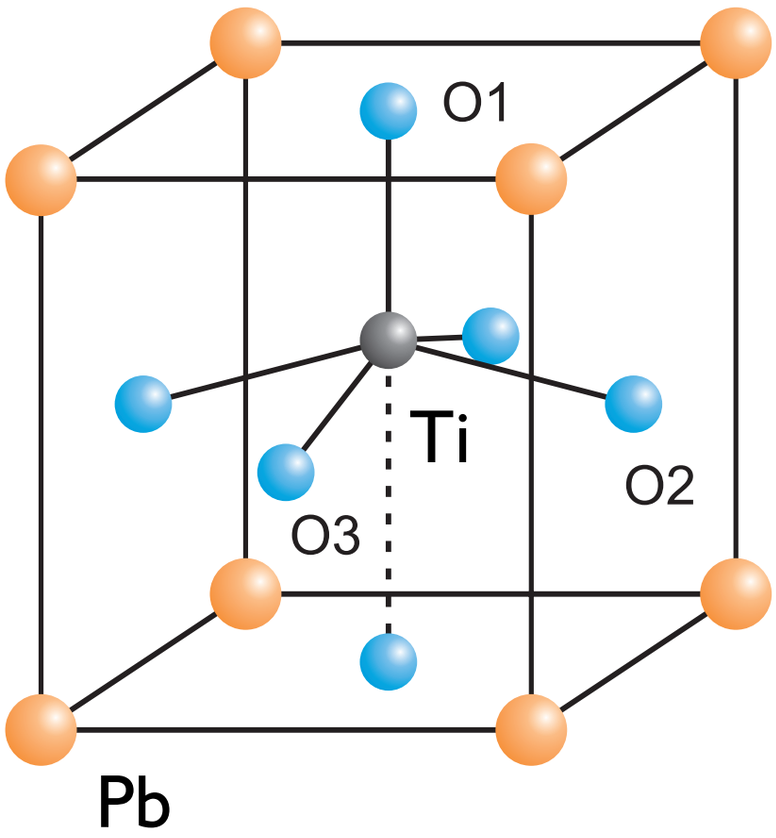


displacement -δ**r**

$$Z^*_{s,\alpha\beta} = \frac{\Omega}{e}\frac{\delta P_\alpha}{\delta r_{s,\beta}} = (2\pi)^{-1}\frac{\delta \Phi_\alpha}{\delta u_{s,\beta}}$$

Tutorial 3: Piezoelectricity

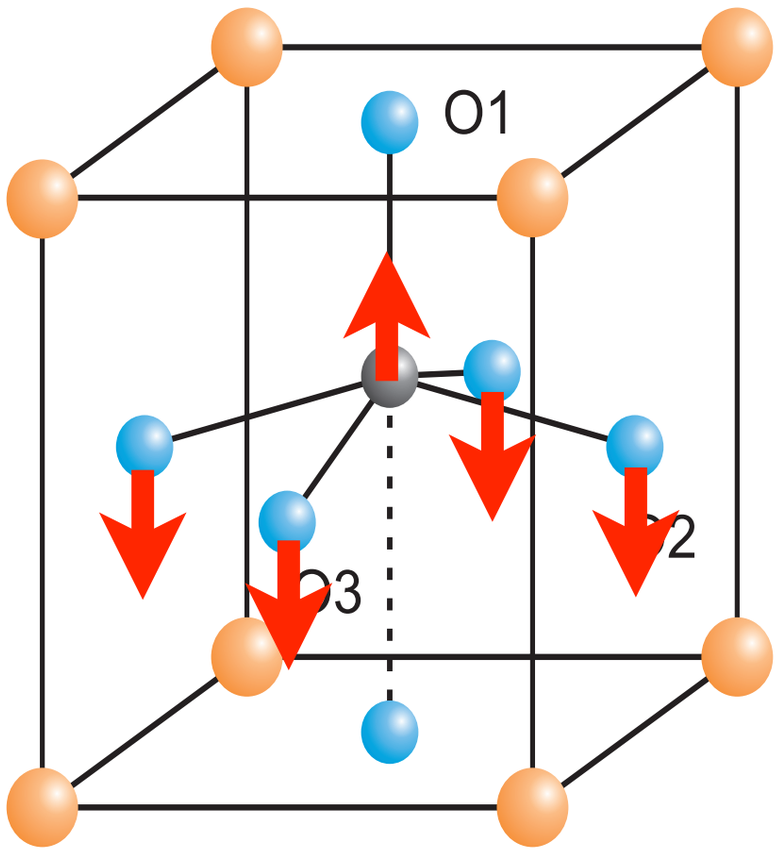
λ_0



tetragonal equilibrium

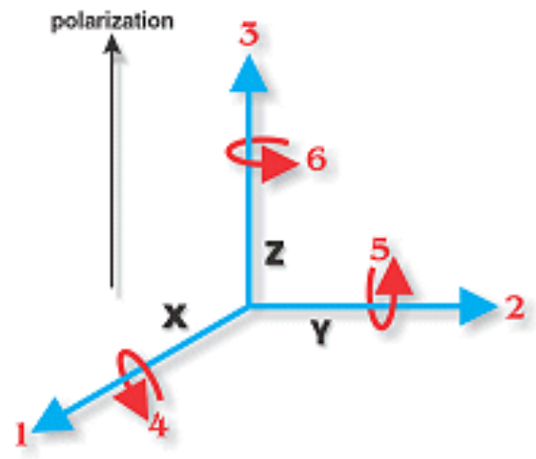
$a_0 = b_0 \neq c_0$

λ_1



tetragonal strained

$a_0 = b_0 \neq c_0(1+\varepsilon_3)$



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https://github.com/spichardo/BerryPI