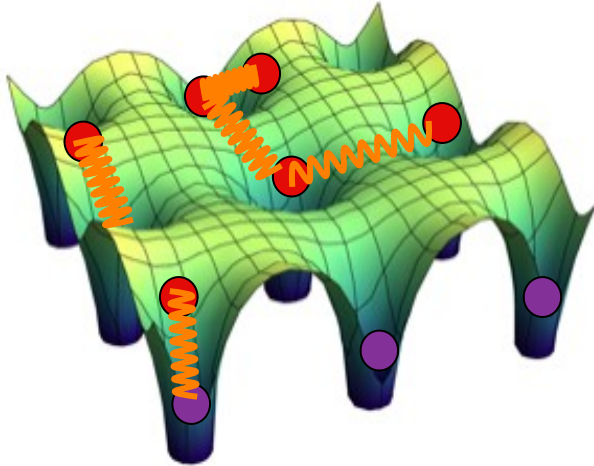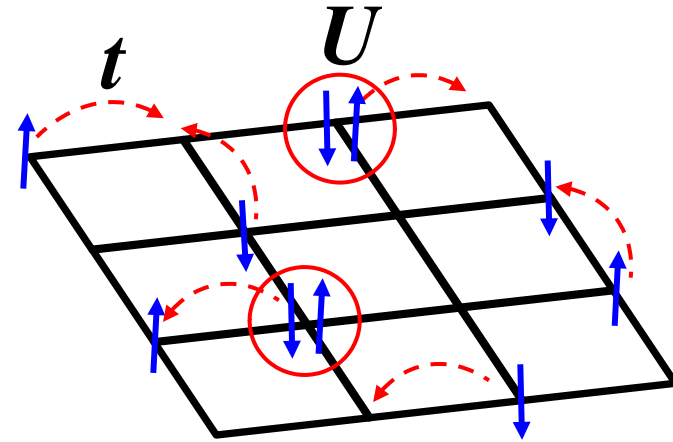# Continuum vs lattice model description

Electrons live in continuum space

$$H = -\frac{\nabla_r^2}{2} + V(\mathbf{r})$$

- r-representation
- ab-initio methods (density functional theory)
- incomprehensible

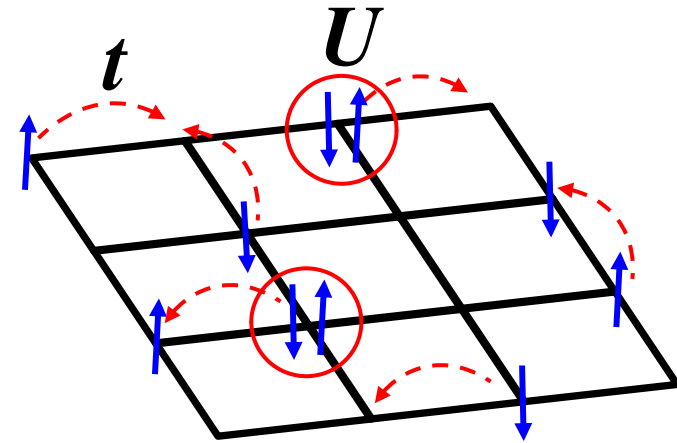Electrons live on discrete lattice (lattice site = atom or orbital)

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- Wannier basis (transition amplitudes)
- quantum field theory (many-body)
- chemical intuition

Continuum vs lattice model description

Take a left turn!

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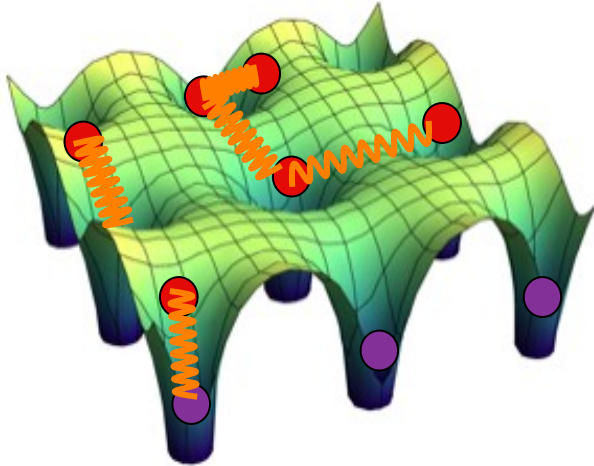
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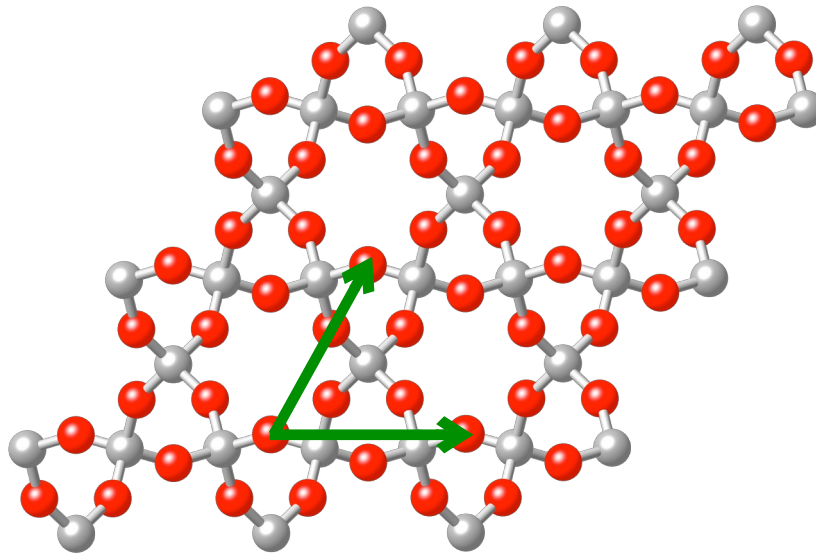- incomprehensible

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Periodic lattice

Crystallographic unit (elementary) cell:

Lattice vectors **a** and **b** are defined by translational symmetry of the crystal
(=> the origin is arbitrary)

The space is filled with unit cells indexed with $\mathbf{R} = n_a \mathbf{a} + n_b \mathbf{b} + \ldots$

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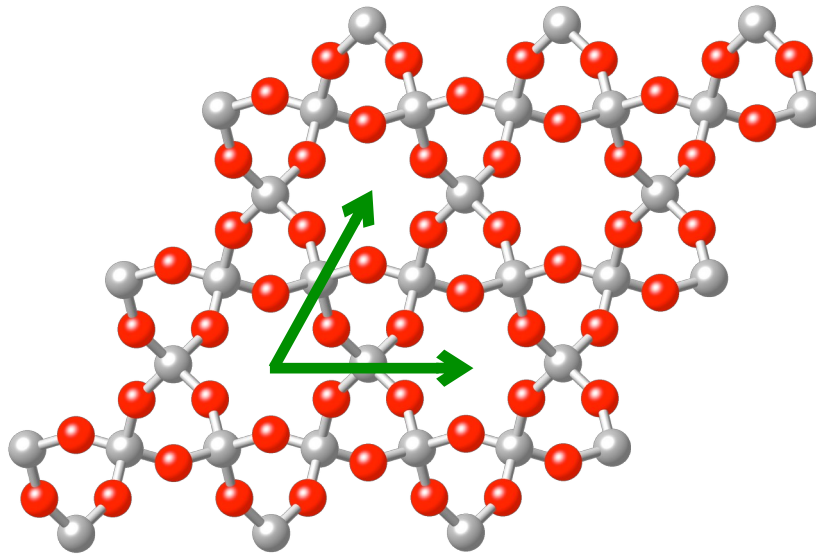

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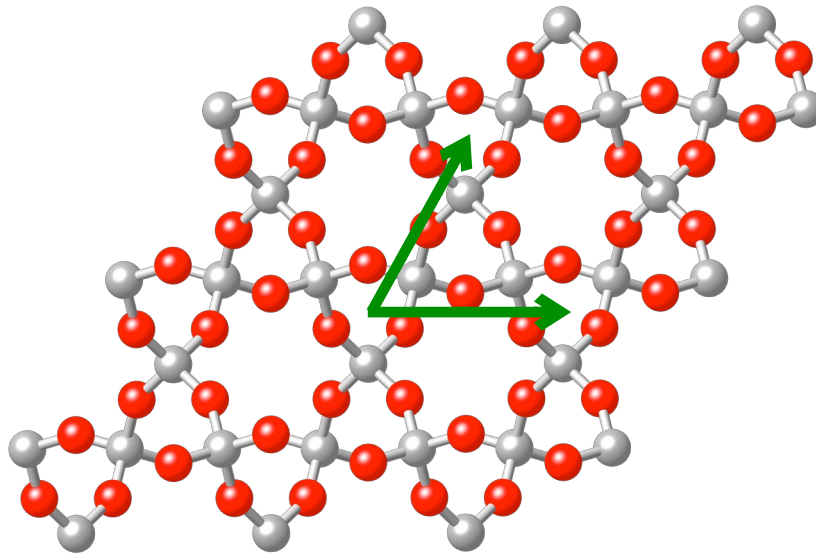

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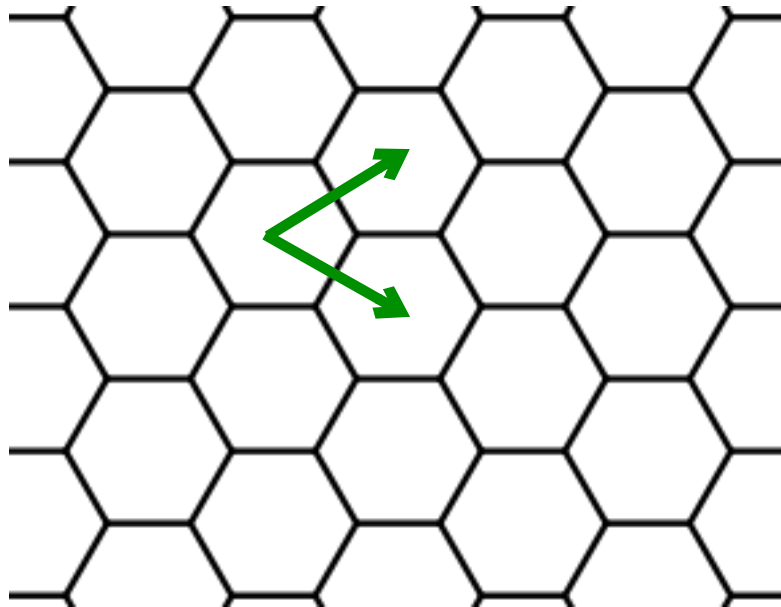

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Bloch theorem (continuum formulation)

Action of the translation operator: $T_{\mathbf{R}}\psi(\mathbf{r}) = \psi(\mathbf{r} - \mathbf{R})$

Different translations commute: $T_{\mathbf{R}_1+\mathbf{R}_2} = T_{\mathbf{R}_1}T_{\mathbf{R}_2}$ (*)

Let us construct common eigenstates of all translation operators (one-dimensional representations of the translation group)

$$T_{\mathbf{R}}\psi(\mathbf{r}) = \alpha(\mathbf{R})\psi(\mathbf{r})$$

(*) implies $\alpha(\mathbf{R}_1 + \mathbf{R}_2) = \alpha(\mathbf{R}_1)\alpha(\mathbf{R}_2)$ and thus $\alpha(\mathbf{R}) = \exp(i\mathbf{k}\cdot\mathbf{R})$

What are the admissible values of **k**?
Periodic boundary conditions: $\psi(\mathbf{r} + N_a\mathbf{a}) = \psi(\mathbf{r}), \quad \psi(\mathbf{r} + N_b\mathbf{b}) = \psi(\mathbf{r}), \ldots$

$$k_a = \frac{1}{|\mathbf{a}|}\frac{2\pi}{N_a} \times 0, 1, \ldots, (N_a - 1)$$

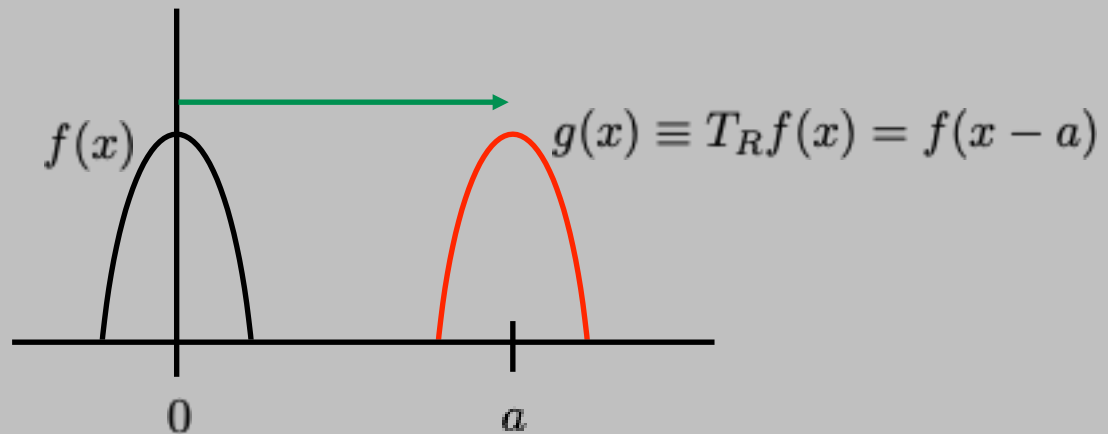Interpretation: **k**=0   functions that are invariant under any translation
        k=π/a   function that change sign under elementary translation

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Let us co

  dimens

$f(x)$ $\qquad\qquad g(x) \equiv T_R f(x) = f(x - a)$

$0 \qquad\qquad a$

(*) impli

What are

Periodic

$k_a = \dfrac{1}{|\mathbf{a}|}$

$T_R : \mathbf{r} \to R\mathbf{r}$

$T_R f(\mathbf{r}) = f(R^{-1}\mathbf{r})$

Interpret

$k = \pi/a$ function that change sign under elementary translation

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Bloch theorem (continuum formulation)

Bloch function:

$$T_{\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{R})\psi_{\mathbf{k}}(\mathbf{r})$$

$$(*)\, \psi_{\mathbf{k}}(\mathbf{r}) = \exp(-i\mathbf{k} \cdot \mathbf{r})u_{\mathbf{k}}(\mathbf{r})$$

periodic function

Bloch functions are orthogonal: $\langle \psi_{\mathbf{k}} | \varphi_{\mathbf{k}'} \rangle \sim \delta_{\mathbf{k}\mathbf{k}'}$

What is it good for?
We have reduced the computational effort immensely!
- from the entire (infinite) crystal to a single unit cell
- from continuum to discrete spectrum

$$(*) \quad T_{\mathbf{R}}[e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r})] = e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})}T_{\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R})}e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r})$$

1st Brillouin zone

Observation:

The vectors **k** and **k**+**G** are equivalent (give the same Bloch state)
=> we do not have to use the primitive cell in the k-space (as long as we
span the same set of inequivalent k-vectors)
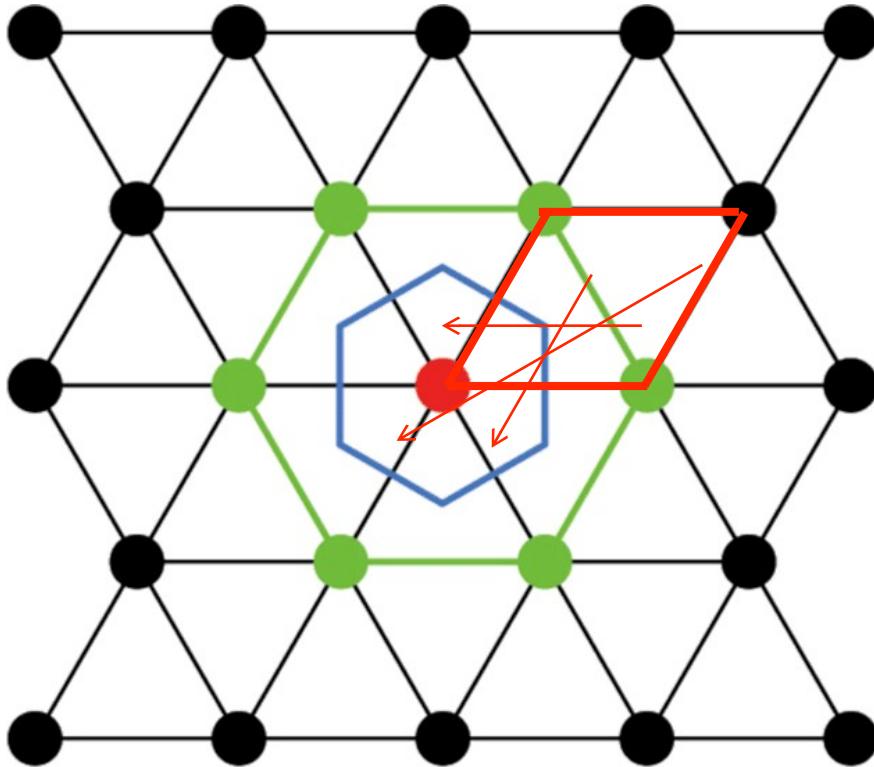
- Woronoi cell of the G-lattice
- one-to-one mapping to primitive cell
- respects point symmetry of the lattice
- standard notation for special points
(solid state codes usually have automated
routines, e.g. xcrysden)

Example:
fcc Brillouin zone
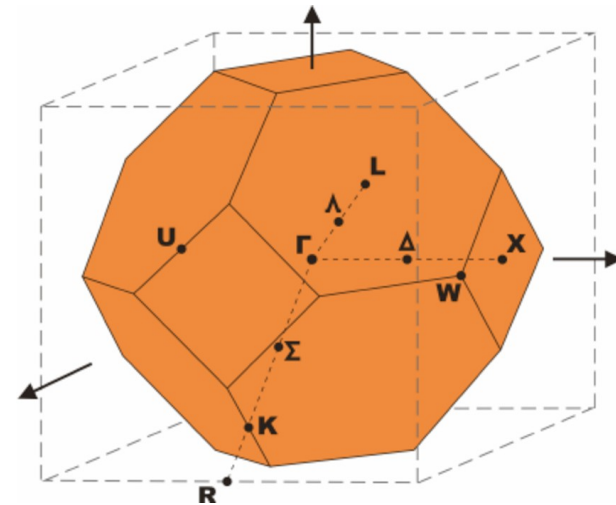
Density of states

Definition: $D(\omega) = \frac{1}{N} \sum_{n,\mathbf{k}} \delta(\omega - \epsilon_{\mathbf{k}n})$

$$= \frac{\Omega}{(2\pi)^3} \sum_n \int_{\text{BZ}} d^3k \quad \delta(\omega - \epsilon_n(\mathbf{k})) = \frac{\Omega}{(2\pi)^3} \sum_n \int_{\epsilon_n(\mathbf{k})=\omega} \frac{dS}{|\nabla_k \epsilon_n(\mathbf{k})|}$$

Remarks:
- Histogram - how many states there are with energies between ω and $\omega + d\omega$
- Allows to calculate quantities that depend only on band energy

$$N_{\text{tot}} = \int d\omega f(\omega) D(\omega)$$ total charge (per unit cell)

$$E = \int d\omega f(\omega) \omega D(\omega)$$ (band) energy (per unit cell)

Calculation:
- histogram (brute force summation over discrete k-mesh
- tetrahedron method (used in standard codes) - linearization of dispersion
- analytic calculation

Density of states

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Calculation:

- histogram (brute force summation over discrete k-mesh)

  'trick': use $\delta(\omega - \epsilon) = -\dfrac{1}{\pi} \text{Im} \lim_{\Gamma \to 0} \dfrac{1}{\omega + \epsilon + i\Gamma}$ and perform the calculation for small finite Γ .

- analytic calculation - band edges (van Hove singularities) $\epsilon(\mathbf{k}) - \epsilon_0 \sim k^2$

  The states with $\epsilon(\mathbf{k}) - \epsilon_0 < \omega$ live in a k-sphere of radius $\omega^{1/2}$
  This gives rise to characteristic
  behavior close to the band edge:

	$N(\omega)$	$D(\omega)$
1D	$\omega^{1/2}$	$\omega^{-1/2}$
2D	ω	1
3D	$\omega^{3/2}$	$\omega^{1/2}$

Example bcc Eu

DoS

Band structure
(spin polarized)

DoS
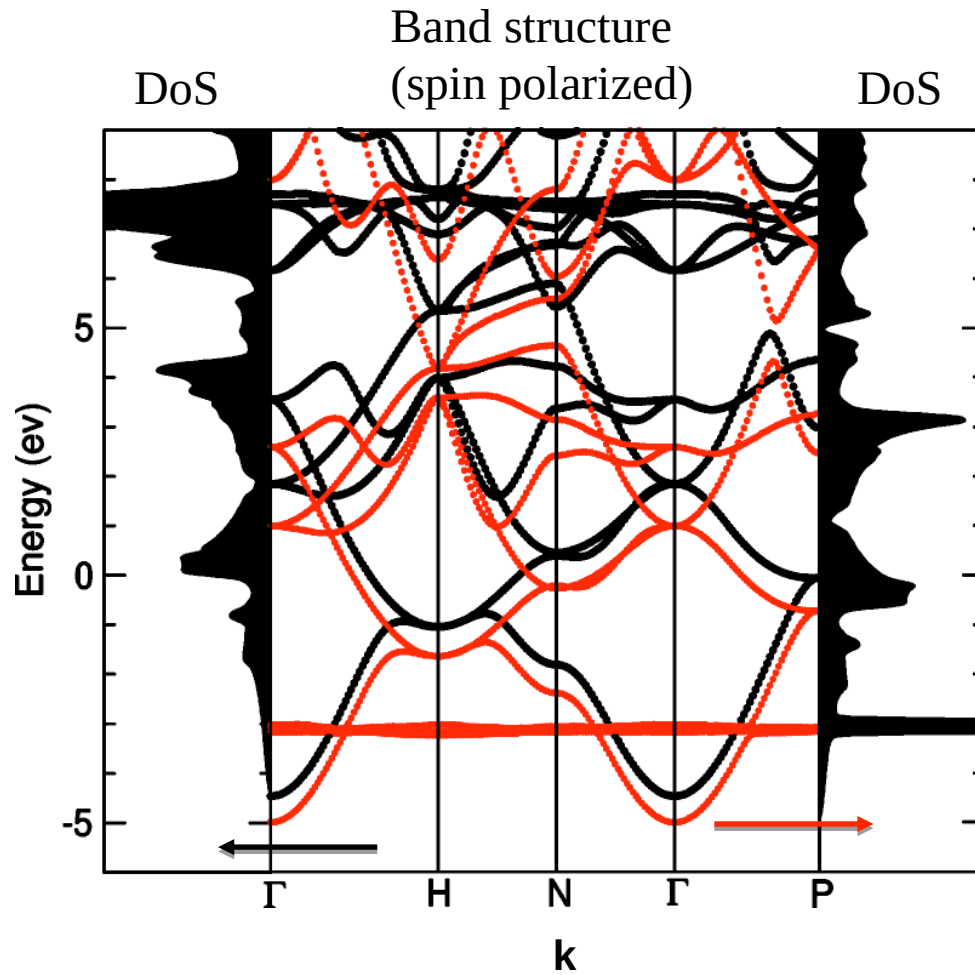
Brillouin zone
bcc (body centred cubic) structure
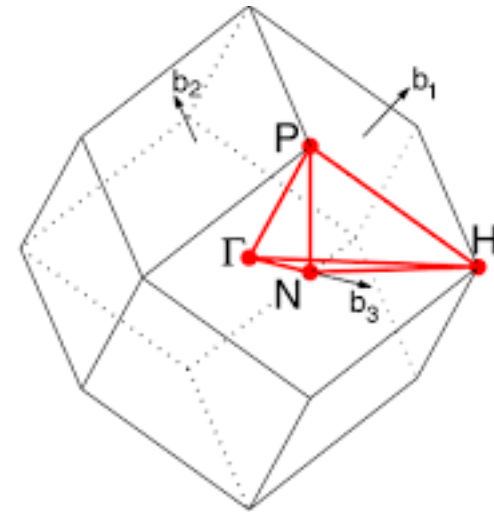
Use of symmetry

Typical symmetries in solids:
- Translation   k-vector (continuous index)   band structure
- Spin SU(2)   S, Sz   magnetic ordering
- Space group   irr. classification of bands.   symmetry protected band crossings
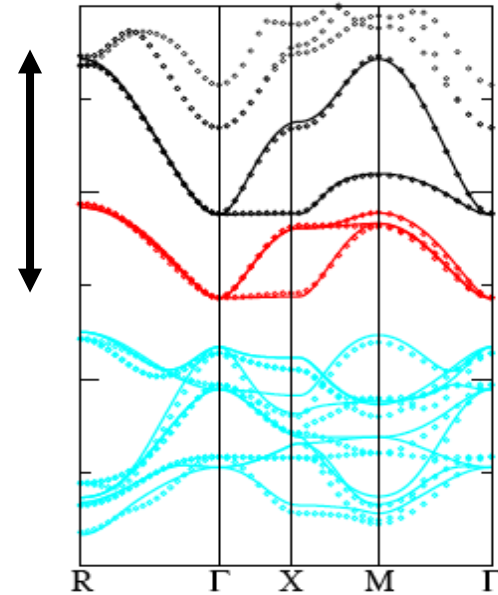- Time reversal

All lead to various selection rules.

Local symmetries:
- Spin SU(2)   S, Sz   atomic multiplets (open shells)
- Point group   irr. classification   local degeneracy, crystal field splitting
- Bond symmetries   selection rules for hopping

Example: cubic crystal field
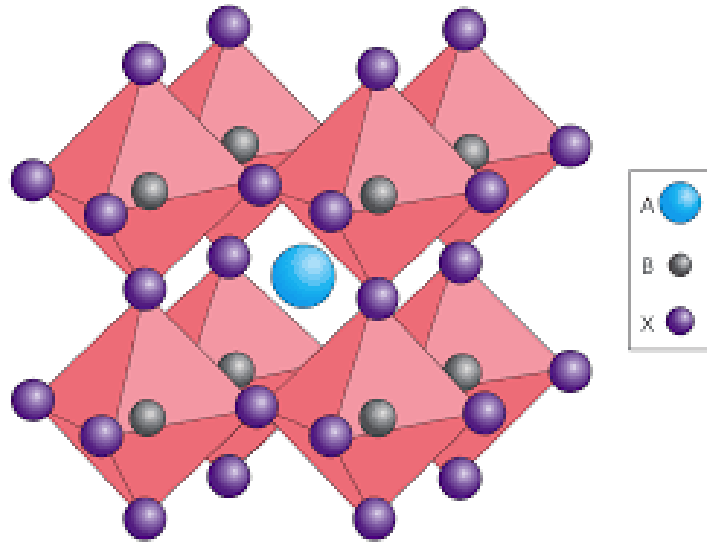
d-orbitals on
the B site

Objective: Construct a lattice model with d-orbitals sitting on the B sites.

On-site Hamiltonian (crystal field)

The B site has a cubic symmetry

The d-orbitals transform like quadratic polynomials x^2, y^2, z^2, xy, xz, yz
(there are only 5 functions because $x^2+y^2+z^2$ is an s-function)

There two irreducible representations:
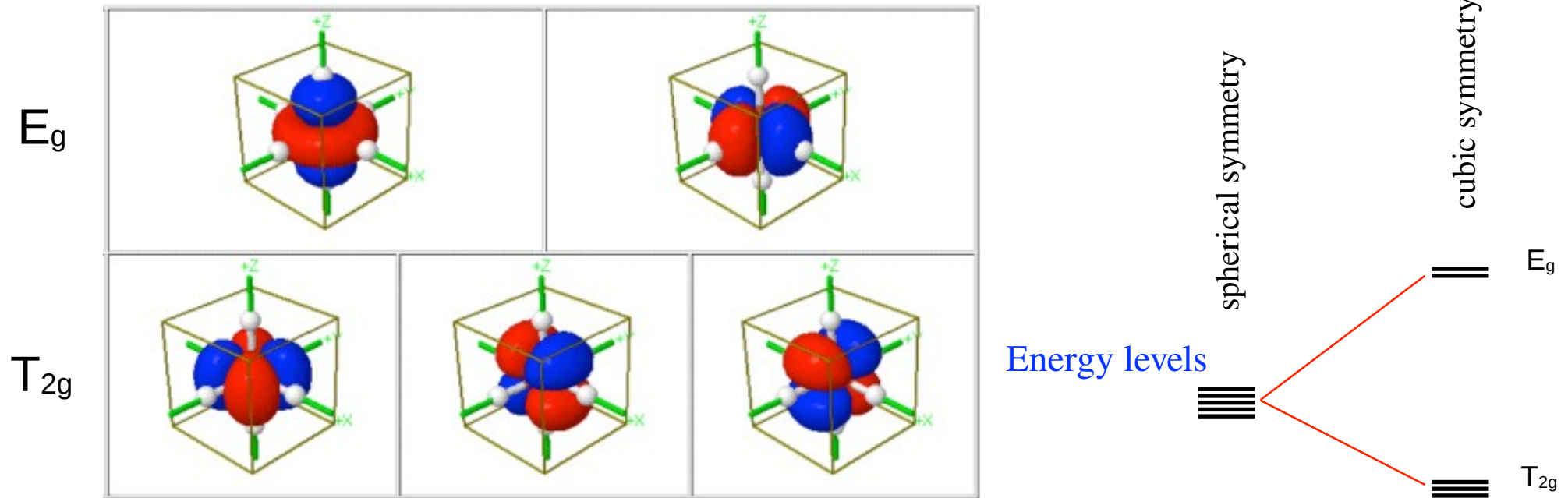
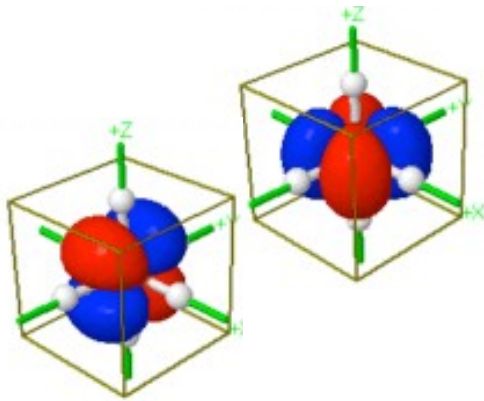# Nearest neighbor hopping

What is the hopping amplitude between these two orbital on neighbor sites?
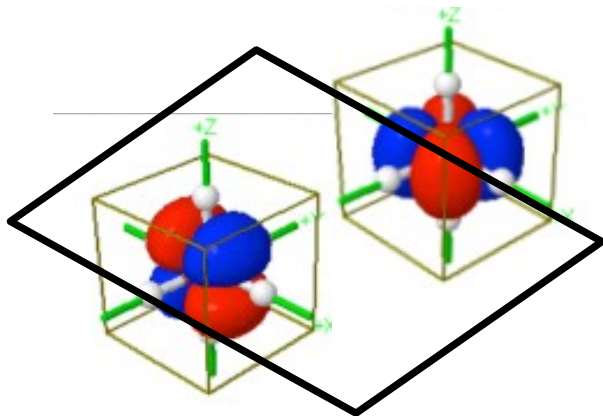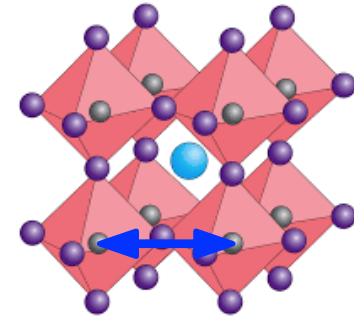
$$\langle \psi_1 | H | \psi_2 \rangle = ?$$

$$\langle \psi_1 | H | \psi_2 \rangle = \langle \hat{\sigma}_x \psi_1 | \hat{\sigma}_x H | \hat{\sigma}_x \psi_2 \rangle$$
$$= \langle \hat{\sigma}_x \psi_1 | H | \hat{\sigma}_x \psi_2 \rangle$$
$$= - \langle \psi_1 | H | \psi_2 \rangle$$
$$\langle \psi_1 | H | \psi_2 \rangle = 0$$

Nearest neighbor hopping

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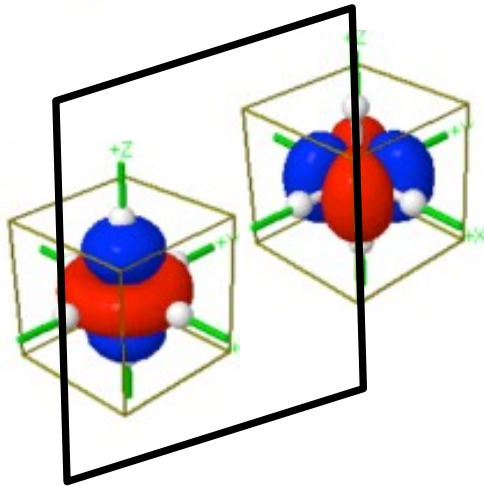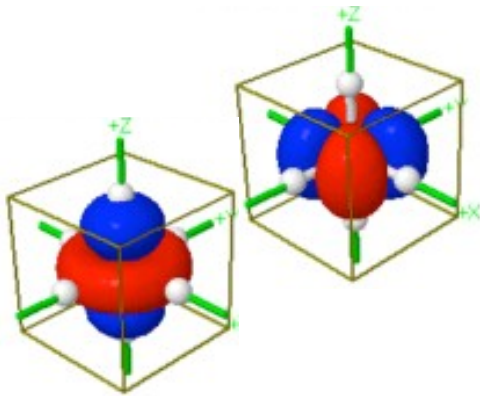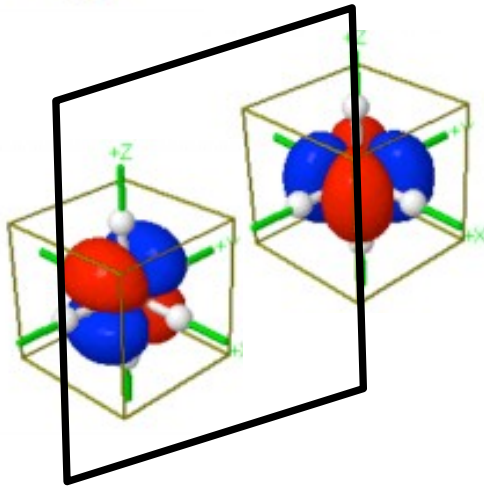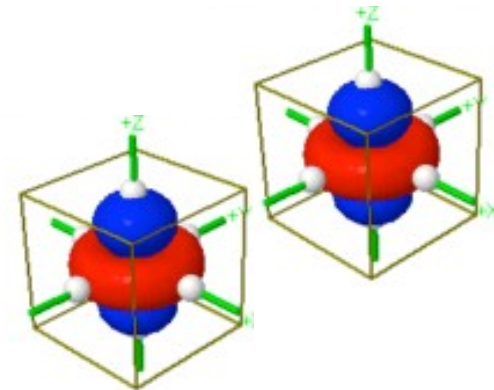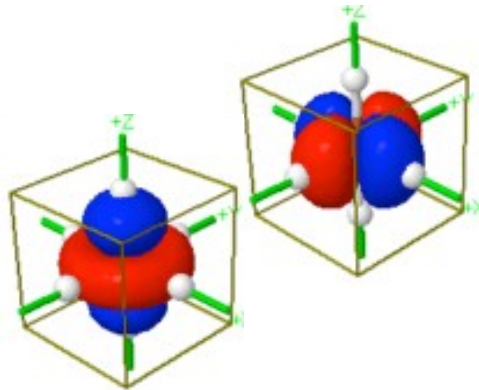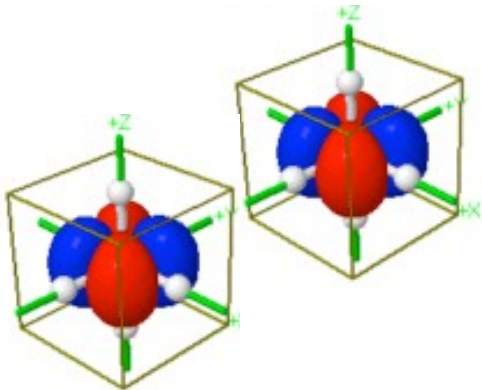
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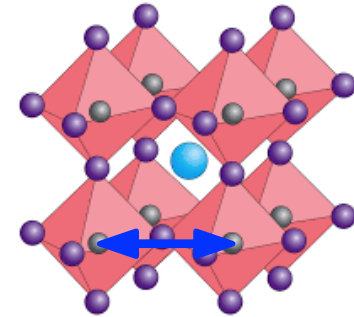
$$
\begin{aligned}
\langle \psi_1 | H | \psi_2 \rangle &= \langle \hat{\sigma}_x \psi_1 | \hat{\sigma}_x H | \hat{\sigma}_x \psi_2 \rangle \\
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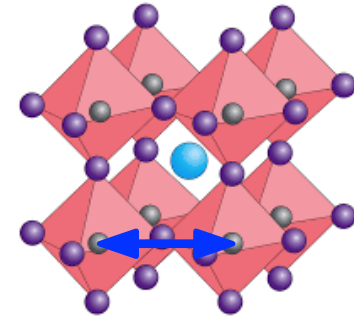$$\langle \psi_1 | H | \psi_2 \rangle = ?$$
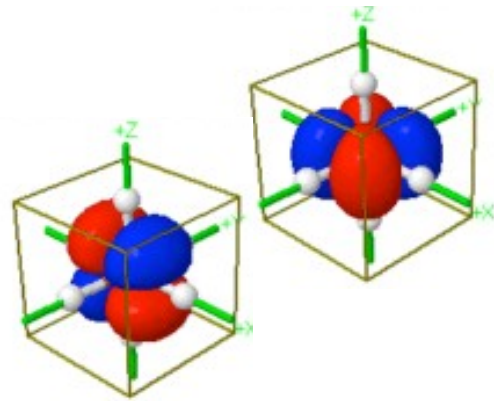
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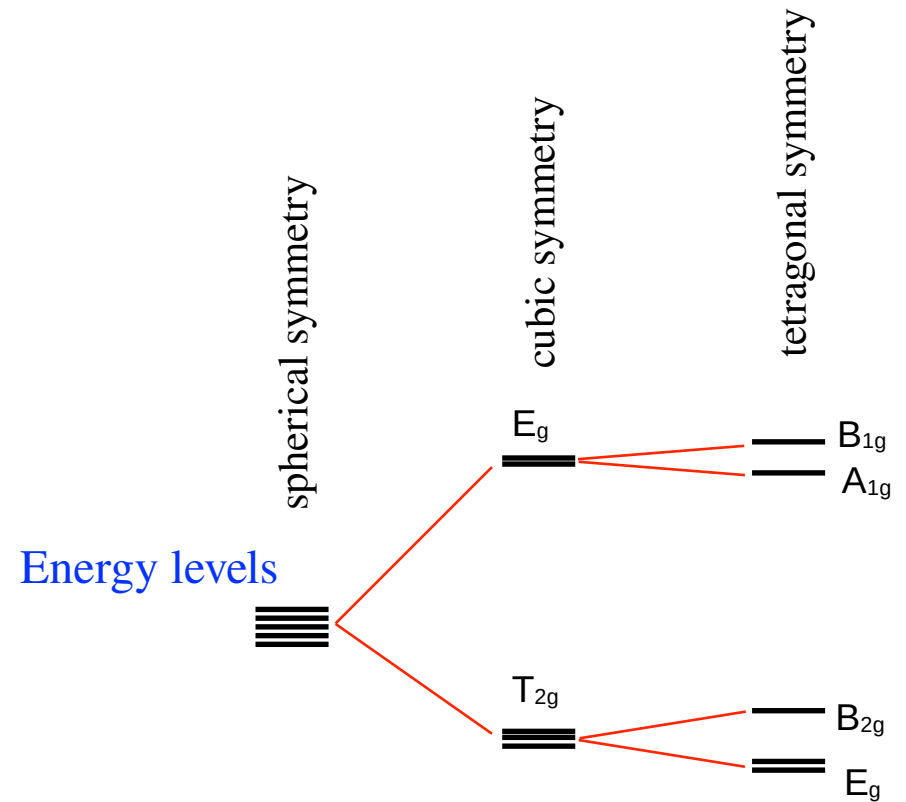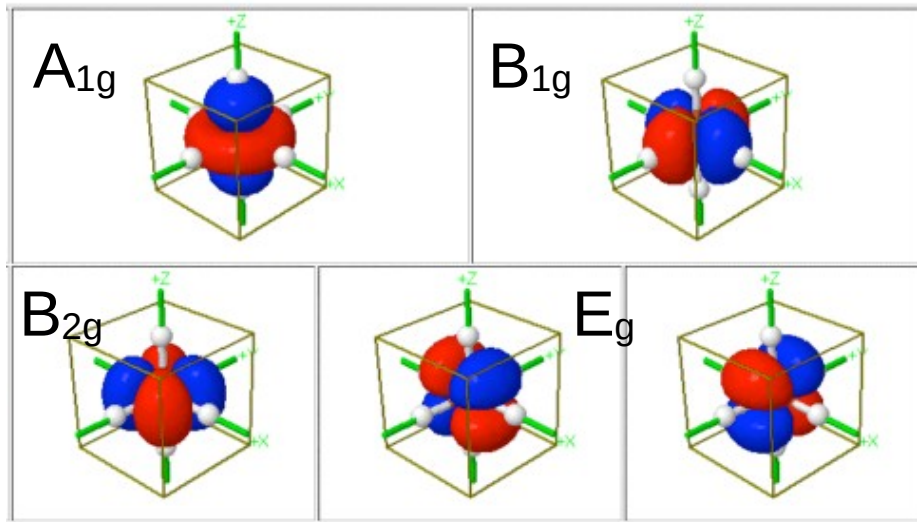$$\langle \psi_1 | H | \psi_2 \rangle = 0$$
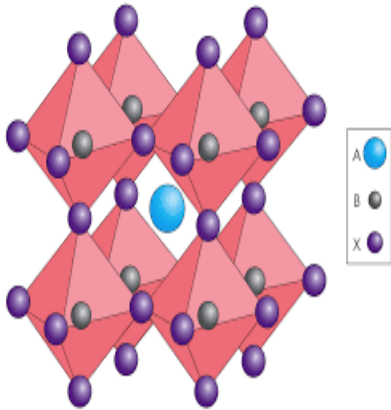
Nearest neighbor hopping

Examples of allowed hopping processes:
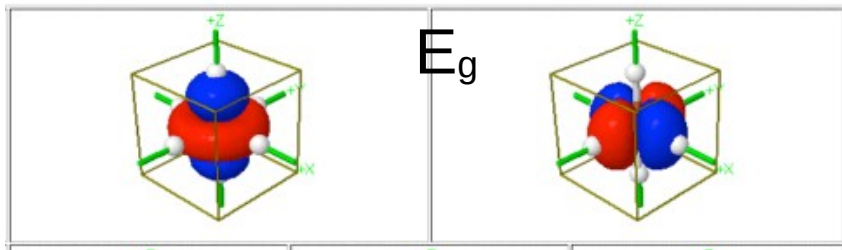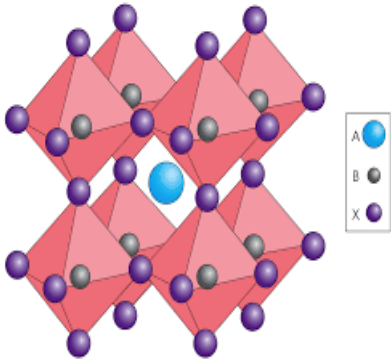
$$\langle \psi_1 | H | \psi_2 \rangle \neq 0$$

Approximate symmetry

Let's us stretch the structure along z-axis a bit
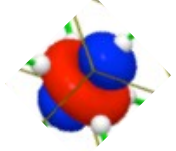=> no cubic symmetry (O$_h$->D$_{4v}$)

A_{1g}

B_{1g}

B_{2g}

E_g

Energy levels

spherical symmetry

cubic symmetry

tetragonal symmetry

E_g

B_{1g}

A_{1g}

T_{2g}

B_{2g}

E_g

Approximate symmetry

Let's us stretch the structure along z-axis a bit
=> no cubic symmetry (O_h->D_{3d})

E_g

A_{1g}

E_g

I cannot draw (find) these

spherical symmetry

cubic symmetry

tetrahedral distortion

Energy levels

E_g

T_{2g}

E_g

E_g

A_{1g}