Electric, magnetic and toroidal polarizations in crystals

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Synopsis

- We consider general order-ℓ electric, magnetic and toroidal multipole densities (called *polarizations*) in crystals; cases with $\ell = 1$ subsume familiar electric dipolarization in ferroelectrics and magnetization in ferromagnets
- Multipole densities defined by symmetry under space inversion i, time inversion θ: signature ss'

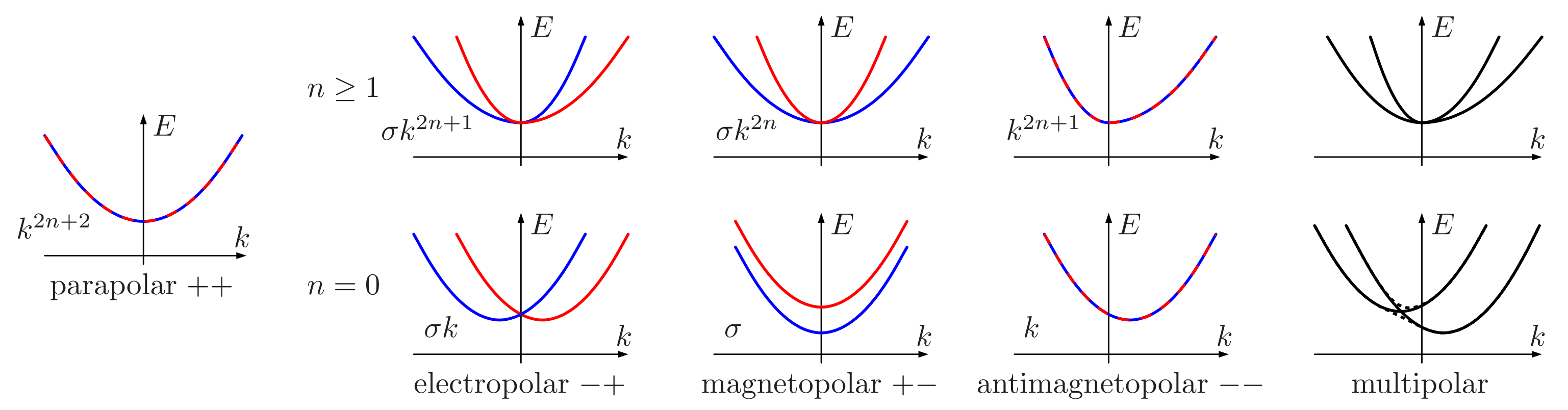
	electric	magnetic	electro-toroidal	magneto-toroidal
ℓ even	$++$	$--$	$-+$	$+-$
ℓ odd	$-+$	$+-$	$++$	$--$

- Five inversion groups with i and θ $\Rightarrow$ five categories of polarized matter

inversion group	symmetry i	θ	$i\theta$	electric ℓ even $++$	electric ℓ odd $-+$	magnetic ℓ even $--$	magnetic ℓ odd $+-$	category of polarized matter
$C_{i\times\theta} = \{e, i, \theta, i\theta\}$	●	●	●	●	○	○	○	parapolar
$C_{\theta} = \{e, \theta\}$	○	●	○	●	●	○	○	electropolar
$C_{i} = \{e, i\}$	●	○	○	●	○	○	●	magnetopolar
$C_{i\theta} = \{e, i\theta\}$	○	○	●	●	○	●	○	antimagnetopolar
$C_{1} = \{e\}$	○	○	○	●	●	●	●	multipolar

- Categories of polarized matter have distinctive spinful electronic band dispersions $E_\sigma(\mathbf{k})$

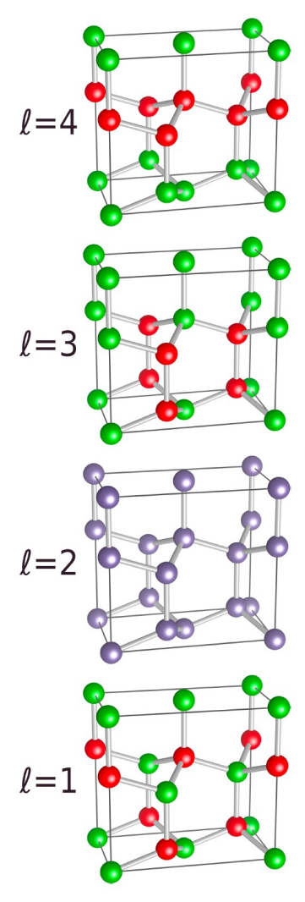
	electric	magnetic
ℓ even	$++: \; k^{2n+2}$	$--: \; k^{2n+1}$
ℓ odd	$-+: \; k^{2n+1}\sigma$	$+-: \; k^{2n}\sigma$



- Multipole densities (polarizations) couple to specific electronic degrees of freedom $\Rightarrow$ identify unique indicators for each multipolar order

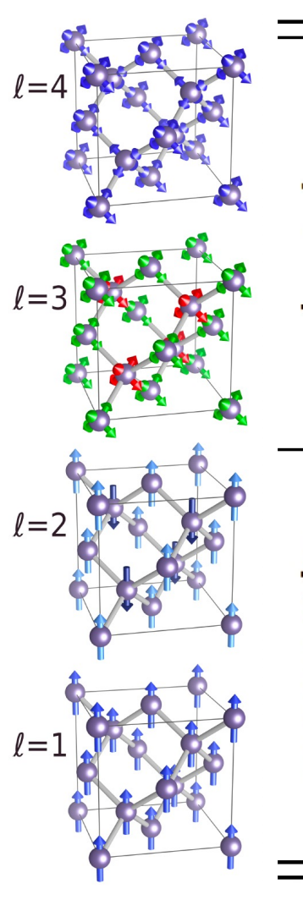
  electric dipolarization $\Rightarrow$ Rashba term; magnetization $\Rightarrow$ Zeeman term

- General and systematic study of polarized versions of lonsdaleite



electric	D_{6h} :	$++$	$\ell = 2$	$m^{(e,2)}(k_x^2 + k_y^2 - 2\,k_z^2)$	lonsdaleite
	D_{3h} :	$-+$	$\ell = 3$	$m^{(e,3)}\,k_z\left[\sigma_x k_x k_y + \tfrac{1}{2}\sigma_y(k_x^2 - k_y^2)\right]$ $+m^{(e,3)}\,\sigma_z\,k_y\,(3k_x^2 - k_y^2)$	
	C_{6v} :	$-+$	$\ell = 1$	$m^{(e,1)}\,(\sigma_x k_y - \sigma_y k_x)$	wurtzite
magnetic	$D_{6h}(D_{3h})$:	$--$	$\ell = 4$	$m^{(m,4)}\,k_x\,(k_x^2 - 3k_y^2)$	
	$D_{6h}(D_{3d})$:	$+-$	$\ell = 3$	$m^{(m,3)}\,\sigma_z k_x k_z\,(k_x^2 - 3k_y^2)$	altermagnet
	$D_{6h}(D_{6})$:	$--$	$\ell = 2$	$m^{(m,2)}\,(k_x^2 - 3k_y^2)(k_y^2 - 3k_x^2)k_x k_y k_z$	
	$D_{6h}(C_{6h})$:	$+-$	$\ell = 1$	$m^{(m,1)}\,\sigma_z$	ferromagnet

- General and systematic study of polarized versions of diamond



electric	O_h :	$++$	$\ell = 4$	$m^{(e,4)}\,(k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)$	diamond
	T_d :	$-+$	$\ell = 3$	$m^{(e,3)}\,\left[\sigma_x k_x(k_y^2 - k_z^2) + \mathrm{cp}\right]$	zincblende
	D_{4h} :	$++$	$\ell = 2$	$m_z^{(e,2)}(k_x^2 + k_y^2 - 2\,k_z^2)$	strain
	C_{3v} :	$-+$	$\ell = 1$	$m^{(e,1)}\,(\sigma_x k_y - \sigma_y k_x)$	zb, piezoelectric
magnetic	$O_h(O)$:	$--$	$\ell = 4$	$m^{(m,4)}[k_x k_y k_z(k_y^2 - k_z^2)(k_z^2 - k_x^2)(k_x^2 - k_y^2)]$	
	$O_h(T_h)$:	$+-$	$\ell = 3$	$m^{(m,3)}[\sigma_x k_y k_z + \mathrm{cp}]$	altermagnet
	$D_{4h}(D_{2d})$:	$--$	$\ell = 2$	$m^{(m,2)}k_z(k_x^2 - k_y^2)$	
	$D_{4h}(C_{4h})$:	$+-$	$\ell = 1$	$m^{(m,1)}\sigma_z$	ferromagnet

Indicators of multipolar order

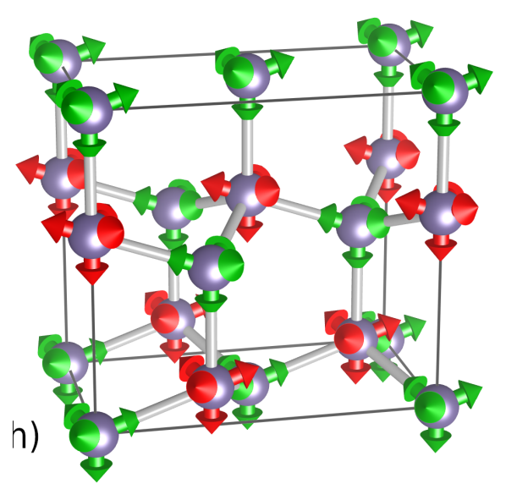
- a multipole density m can be decomposed into components m_α^G associated with IRs α of the crystallographic point group G
- theory of invariants: effect of m described by terms $\sum_\alpha a_\alpha^G K_\alpha^G m_\alpha^G$ in Hamiltonian H, where tensors K_α^G have same signature ss' as m_α
- finite expectation value of indicator $I_\alpha^G = a_\alpha^G K_\alpha^G$ signals polarization m_α^G
- examples: expectation value of σ_z signals magnetization $m^{(m,1)}$; expectation value of $\sigma_x k_y - \sigma_y k_x$ signals electric dipolarization $m^{(e,1)}$

Toroidal moments are not distinct in crystals

- electric, magnetic and toroidal moments can be distinguished in vacuum
- in crystals, all multipoles map onto the same finite set of IRs of G
- allowed toroidal moment couples to same indicator as allowed electric or magnetic multipole with same ss' $\Rightarrow$ same observable physics!

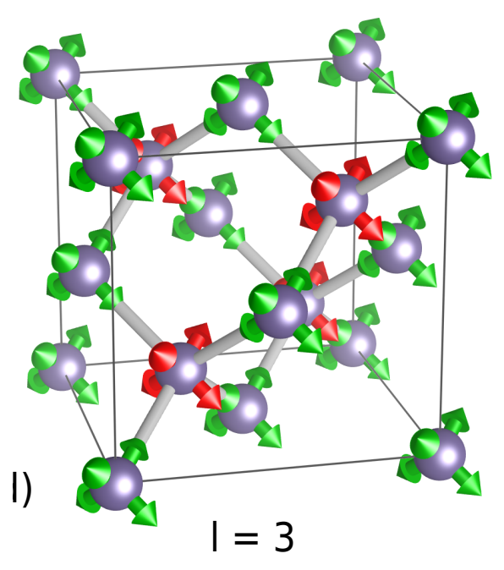
Electropolarizations: Rashba and Dresselhaus terms

Lonsdaleite structure with electric dipolarization: wurtzite



- site symmetry C_{3v} allows local electric octupoles; with different atoms on red/green sites $\Rightarrow$ dipolarization
- Rashba term is associated invariant (indicator)

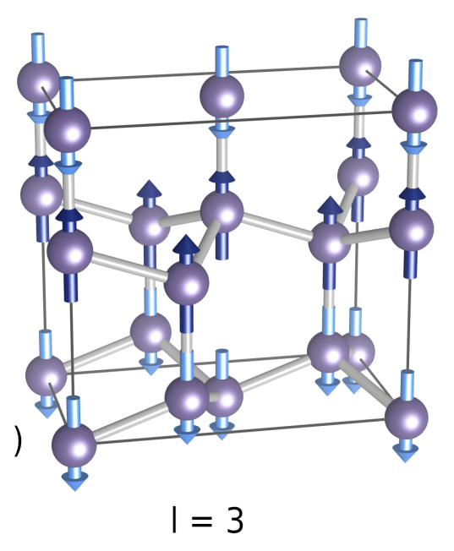
Diamond structure with electric octupolarization: zincblende



- site symmetry T_d allows local electric octupoles; with different atoms on red/green sites $\Rightarrow$ octupolarization
- Dresselhaus term is associated invariant (indicator)

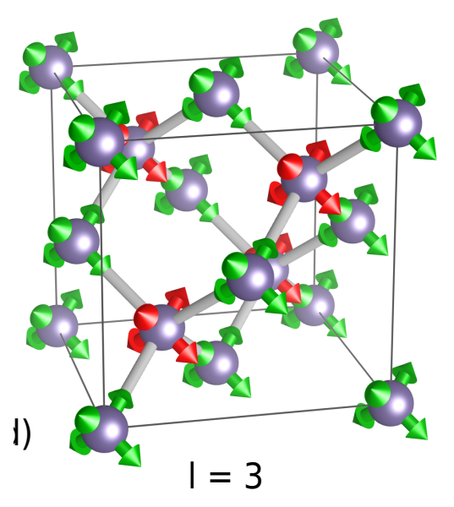
Magnetic octupolarization: Magnetopolar AFM

Lonsdaleite structure with magnetic octupolarization



- local magnetic dipoles forming a centrosymmetric AFM
- octupolarization indicator $\propto \sigma k^4$: 'g-wave' altermagnet

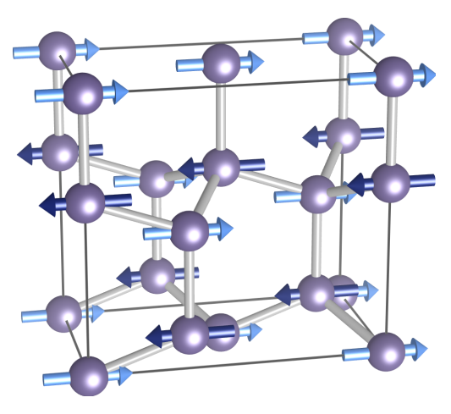
Diamond structure with magnetic octupolarization



- local magnetic octupoles ordered ferroically
- octupolarization indicator $\propto \sigma k^2$ with cubic symmetry: 'd-wave' altermagnet w/o global spin-quantization axis

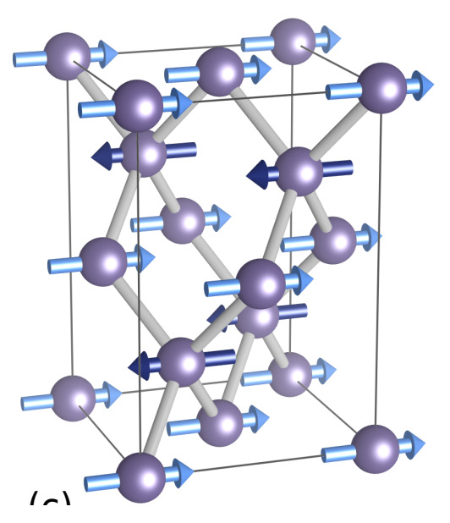
Magnetic quadrupolarization: Antimagnetopolar AFM

Lonsdaleite structure with magnetic quadrupolarization



- Néel vector $\parallel c$: quadrupolarization indicator $\propto k^7$
- Néel vector $\perp c$: quadrupolarization indicator $\propto k$

Diamond structure with magnetic quadrupolarization



- bulk diamond AFM: quadrupolarization indicator $\propto k^3$
- with strain/quantum confinement $\perp$ Néel vector: $\propto k$

Read more details in our publication!

preprint arXiv:2301.09842, to appear in Physical Review B

part of *Collection in Honor of Emmanuel I. Rashba and His Fundamental Contributions to Solid-State Physics*