Electric, magnetic and toroidal polarizations in crystals

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We consider general order-$l$ electric, magnetic and toroidal multipole densities (called polarizations) in crystals; cases with $l = 1$ subsume familiar electric dipolarization in ferroelectrics and magnetization in ferromagnets.

Multipole densities defined by symmetry under space inversion $i$, time inversion $\theta$: signature $s_s$.

Five inversion groups with $i$ and $\theta \Rightarrow$ five categories of polarized matter.

<table>
<thead>
<tr>
<th>Inversion Group</th>
<th>Symmetry $s_s$</th>
<th>Electric Order $l$</th>
<th>Magnetic Order $l$</th>
<th>Category of Polarized Matter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{i\theta}$</td>
<td>$s_s$</td>
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<td>$l$ odd</td>
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Categories of polarized matter have distinctive spinful electronic band dispersions $E_s(k)$.

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Indicators of multipolar order

A multipole density $m$ can be decomposed into components $m_{\alpha}^L$ associated with IRs $\alpha$ of the crystallographic point group $G$.

Theory of invariants: effect of $m$ described by terms $\sum_{\alpha} a_\alpha^L K^\alpha m_{\alpha}^L$ in Hamiltonian $H$, where tensors $K^\alpha$ have same signature $s_s$ as $m_{\alpha}$.

Finite expectation value of indicator $I_{\alpha} = a_\alpha^L K^\alpha$ signals polarization $m_{\alpha}^L$.

Examples: expectation value of $\sigma z$ signals magnetization $m_z$, expectation value of $\sigma_x k_y - \sigma_y k_x$ signals electric dipolarization $m_{xy}$.

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 $s_s$.

Electropolarizations: Rashba and Dresselhaus terms

Lonsdaleite structure with electric dipolarization: wurtzite

Site symmetry $C_{i\theta}$ 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).

Synopsis

- Multipole densities (polariations) 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.

General and systematic study of polarized versions of diamond.

Magnetic octupolarization: Magnetopolar AFM

Lonsdaleite structure with magnetic octupolarization

- Local magnetic dipoles forming a centrosymmetric AFM.
- Octupolarization indicator $\propto \sigma k^4, \cdot g$-wave alternmagnet.

Diamond structure with magnetic octupolarization

- Local magnetic octupoles ordered ferroically.
- Octupolarization indicator $\propto \sigma k^2$ with cubic symmetry: "d-wave" alternmagnet w/o global spin-quantization axis.

Magnetic quadrupolarization: Antimagnetopolar AFM

Lonsdaleite structure with magnetic quadrupolarization

- Néel vector $\parallel c$: quadrupolarization indicator $\propto k^2$.
- Néel vector $\perp c$: quadrupolarization indicator $\propto k$.

Diamond structure with magnetic quadrupolarization

- Bulk diamond AFM: quadrupolarization indicator $\propto k$.
- With strain/quantum confinement $\perp$ Néel vortex $\propto k$.

Read more details in our publication!

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