Non-Linear Hall Effect in Flatlands and Chiral Crystals

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Acknowledgments

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Discussions:
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M. Deshmukh (TIFR)

Pancharatnam-Berry Phase

- Adiabatic evolution of a quantum state

$$|\Psi_n(t)\rangle = e^{i\gamma_n(t)} e^{-\frac{i}{\hbar}\int_0^t dt'\,\varepsilon_n(R(t'))} |n(R(t))\rangle$$

- Geometric phase can arise

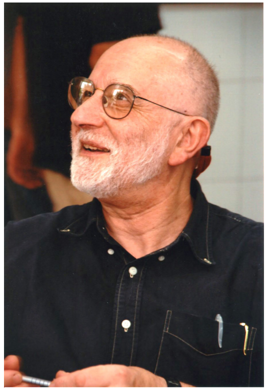
$$\gamma_n(t) = i\int_0^t \langle n(R(t'))|\frac{d}{dt'}|n(R(t'))\rangle$$

$$= i\int_{R(0)}^{R(t)} dR\langle n(R)|\nabla_R|n(R)\rangle$$

- Can define a connection and a curvature

$$\mathcal{A}_n(R) = i\langle n(R)|\nabla_R|n(R)\rangle \qquad \Omega_n(R) = \nabla_R \times \mathcal{A}_n(R)$$

S. Pancharatnam
(1934-1969)



M. V. Berry
(1941-)

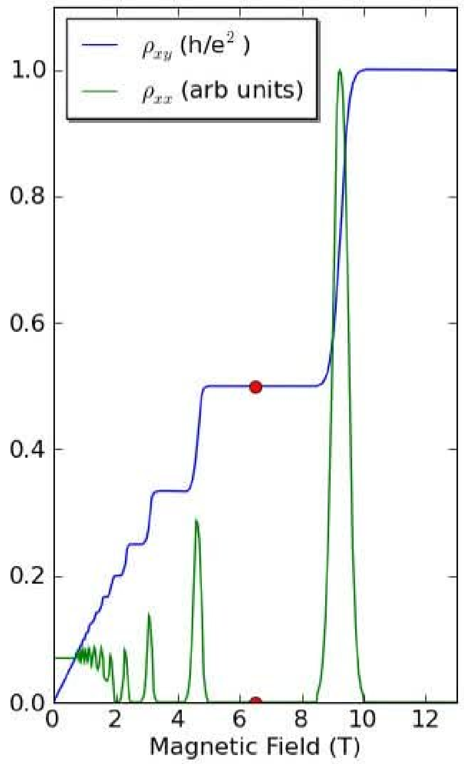
Berry curvature and quantum Hall effect

- Pancharatnam-Berry phases underpin many diverse quantum phenomena

- Celebrated quantum Hall effect

$$\sigma_{ab} = -\frac{e^2}{\hbar}\varepsilon_{abc}\int \frac{d^n k}{(2\pi)^n}\Omega_c f_0$$

- Need to break time reversal symmetry



Berry Curvature Dipole and Non-Linear Hall Effect

- Usual (linear) Hall effect vanishes in time reversal invariant systems
- Time-reversal invariant systems with low-enough symmetry can show non-linear Hall effect

  Sodemann and Fu, Phys. Rev. Lett. 115, 216806 (2015)

- Second-order response

$$\chi_{abc} = -\frac{e^3\tau}{2(1+i\omega\tau)}\varepsilon_{adc}\int \frac{d^n k}{(2\pi)^n}(\partial_b \Omega_d) f_0$$

$$\partial_a = \partial / \partial k_a$$

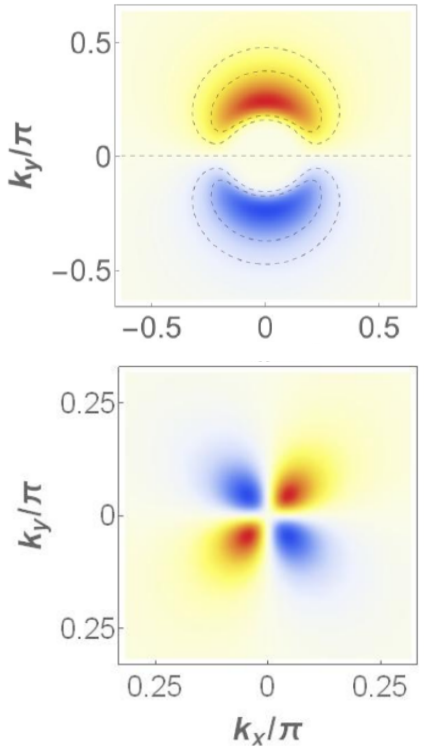
Berry Curvature Dipole and Non-Linear Hall Effect

- Underlying origin is the first-order moment of Berry curvature: Berry curvature dipole

$$D_{ab} = \int \frac{d^n k}{(2\pi)^n} (\partial_a \Omega_b) f_0$$

$$\partial_a = \partial / \partial k_a$$

- Can be generalized to higher order moments



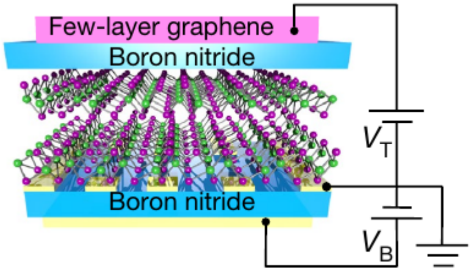
Roy and Narayan,
J. Phys.: Condens. Matter 35, 385301 (2022)

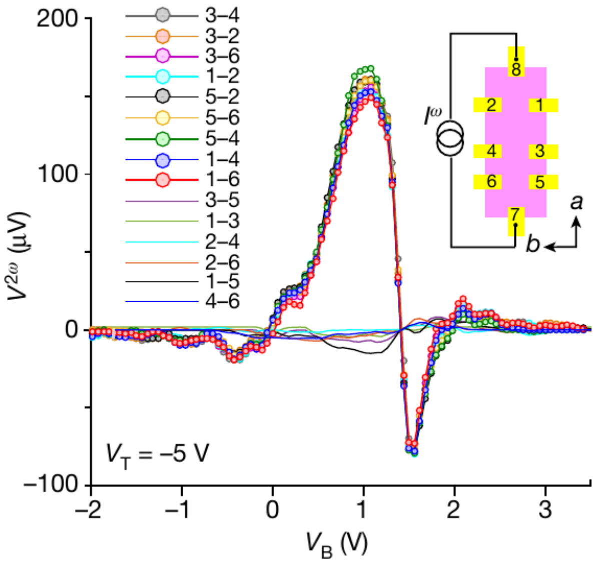
Non-Linear Hall Effect: Experimental Realization I

- First experimental realization in bilayer and few-layer WTe_2

  Ma *et al.*, Nature 565, 337 (2019)

  Kang *et al.*, Nature Materials 18, 324 (2019)

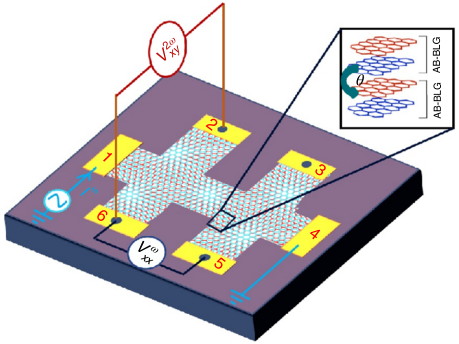




- Dual gated geometry measures voltage response at 2ω, when current applied at ω

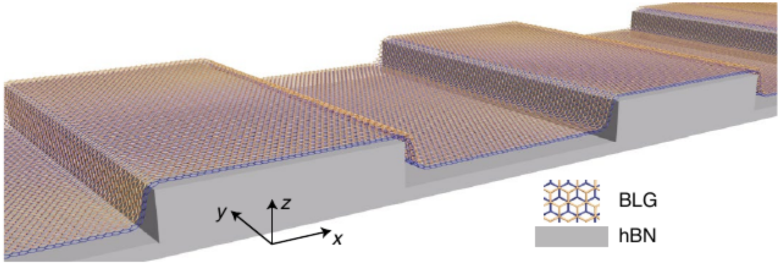
Non-Linear Hall Effect: Experimental Realization II

Twisted double bilayer graphene



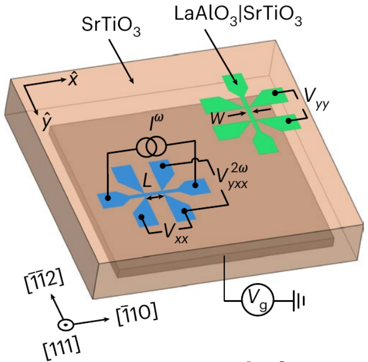
Sinha *et al.*, Nature Physics 18, 765 (2022)

Artificially corrugated graphene



Ho *et al.*, Nature Electronics 4, 116 (2021)

Oxide interfaces

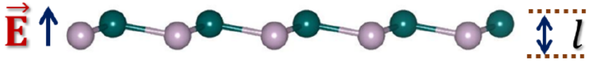


Lesne *et al.*, Nature Materials 22, 576 (2023)

Recent review:
Bandyopadhyay, Joseph, and Narayan,
Materials Today Electronics 8, 100101 (2024)

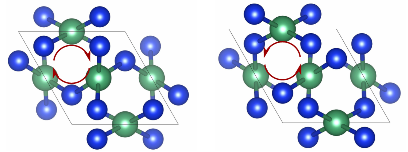
Plan for this talk

Graphene analogs: Silicene, Germanene and Stanene



Bandyopadhyay, Joseph, and Narayan,
2D Materials 9, 035013 (2022)

Chiral Materials: Metals, semimetals and semiconductors

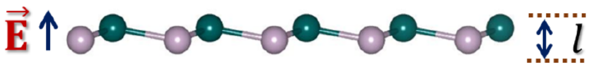


Joseph, Bandyopadhyay, and Narayan,
Chemistry of Materials, in press (2024)

Focus on the intrinsic contribution only!

Plan for this talk

Graphene analogs: Silicene, Germanene and Stanene



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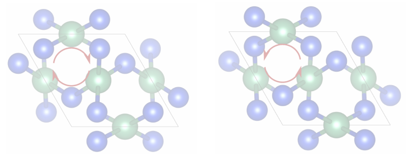
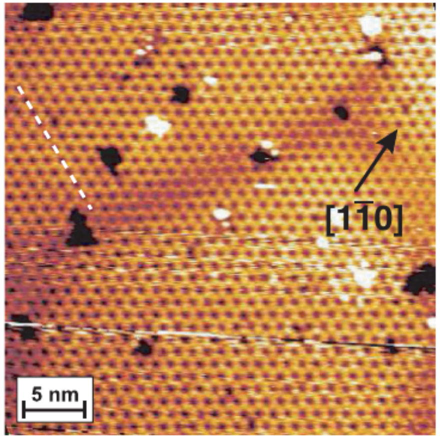
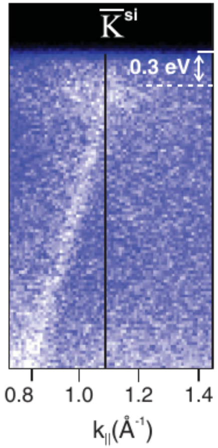


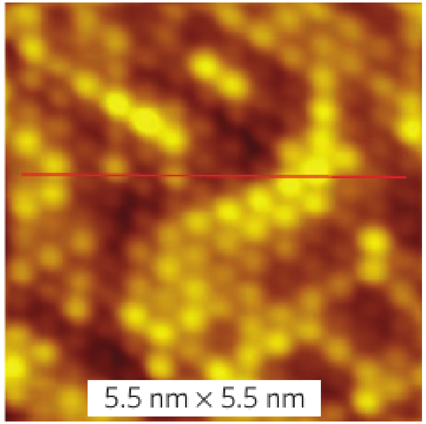
Joseph, Bandyopadhyay, and Narayan,
Chemistry of Materials, in press (2024)

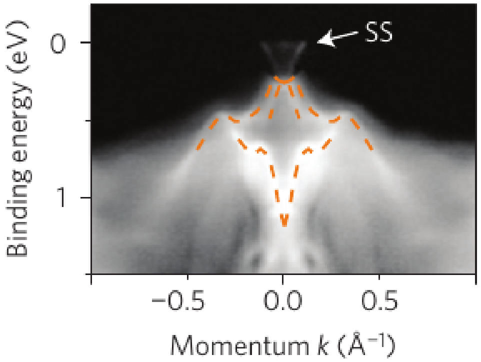
Graphene Analogs: Silicene, Germanene, Stanene





Vogt *et al.*, Phys. Rev. Lett. 108, 155501 (2012)

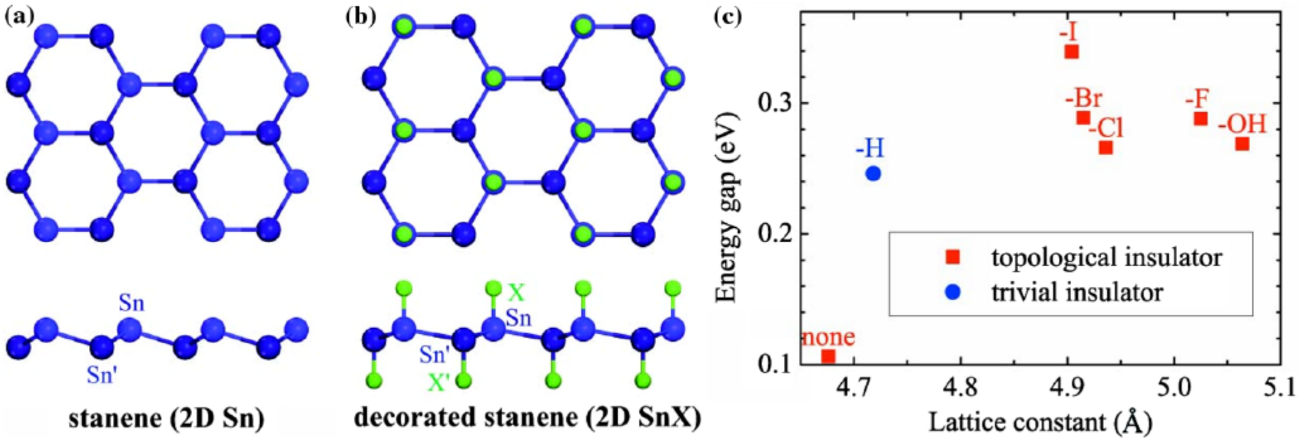




Zhu *et al.*, Nature Materials 14, 1020 (2015)

- Possible signatures of two-dimensional variants of Si, Ge and Sn
- Honeycomb structure, but not planar
- Potential to exploit larger spin orbit coupling than graphene

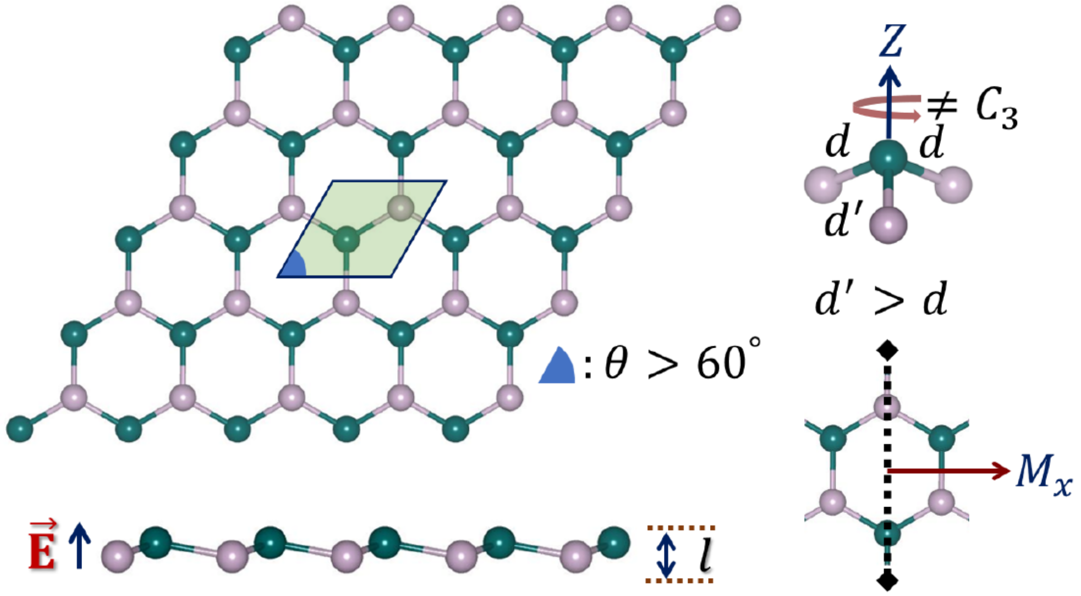
Topology of silicene, germanene, stanene



Xu *et al.*, Phys. Rev. Lett. 111, 136804 (2013) Ezawa, JPSJ 84, 121003 (2015)

- Topologically non-trivial nature theoretically identified early on
- Unambiguous measurement of edge states still awaited

Buckled Honeycomb Layers: Symmetries



- Maximum permitted symmetry for finite BCD in 2D: single mirror line
- Apply uniaxial strain to remove C_3 and two σ_d reflection symmetry planes
- Electric field breaks inversion symmetry

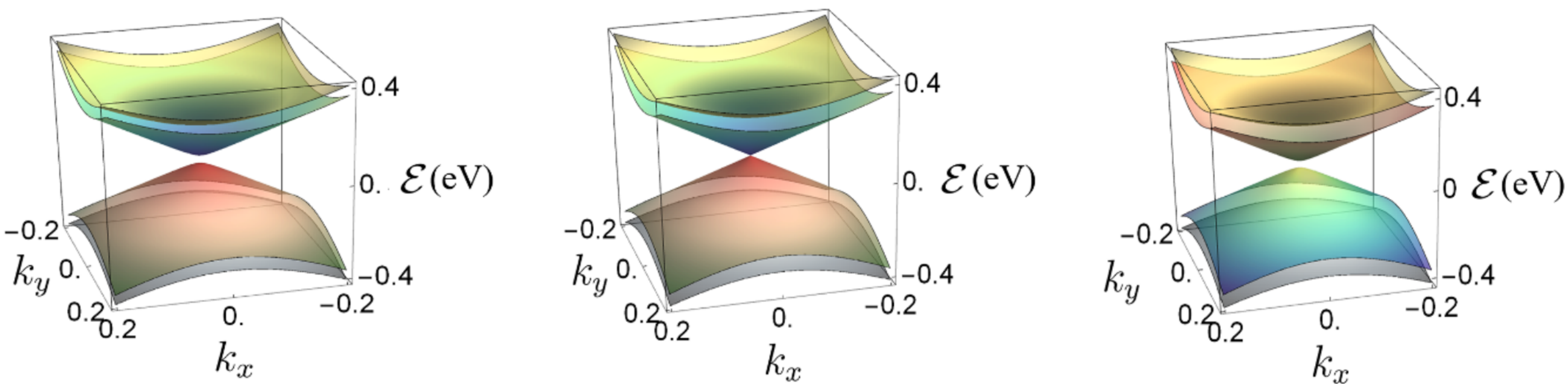
Buckled Honeycomb Layers: Tight-binding model

$$\hat{H} = -t \sum_{\langle ij \rangle, \sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + i \frac{\lambda_{SO}}{3\sqrt{3}} \sum_{\langle\langle ij \rangle\rangle, \sigma} \sigma \zeta_{ij} c_{i,\sigma}^{\dagger} c_{j,\sigma} - l \sum_{i,\sigma} \nu_i E_z c_{i,\sigma}^{\dagger} c_{i,\sigma}.$$

- Silicene, germanene, stanene can be described by same model with different values of the parameters
- Kane-Mele type of spin orbit coupling
- Electric field resulting in staggered sublattice potential
- Tight-binding results cross-checked with density functional computations

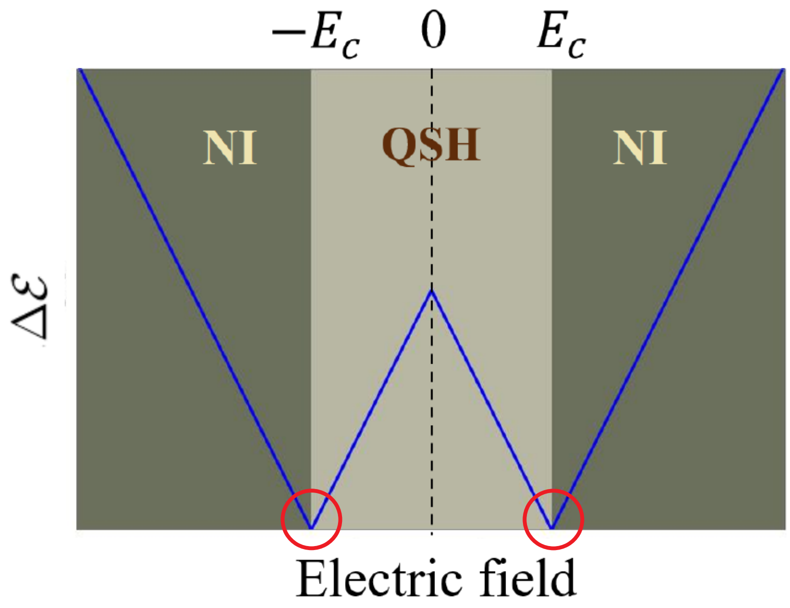
Buckled Honeycomb Layers: Electric Field Tunable Topology

Increasing *E*



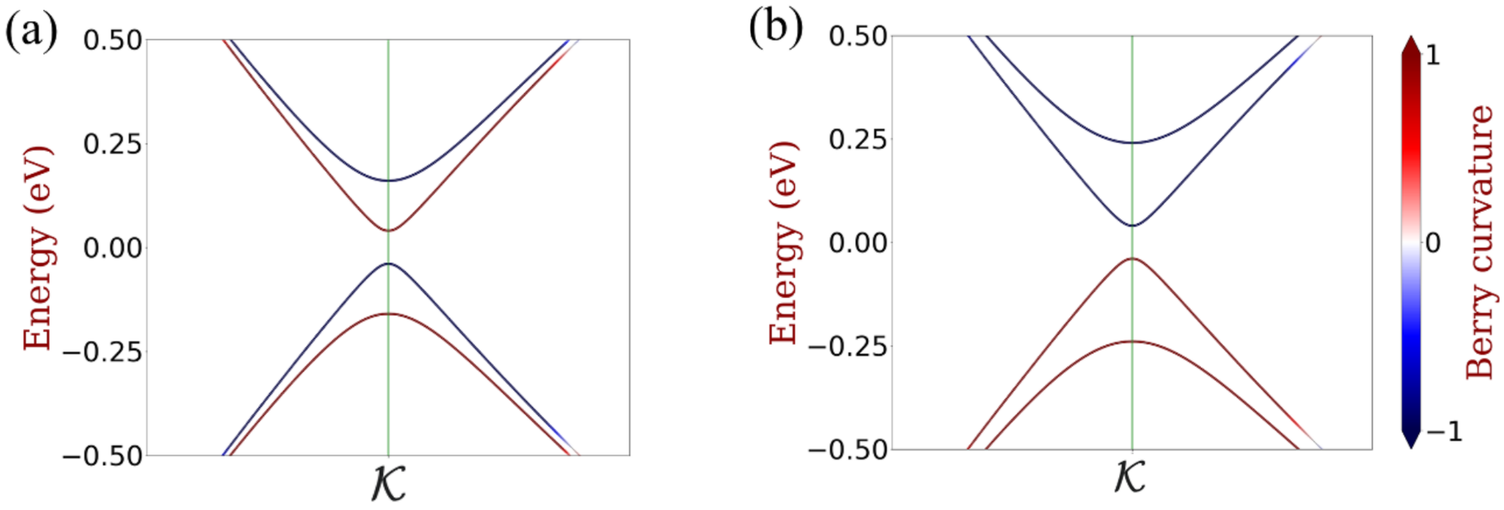
- Electric field strongly controls the band structure
- Quantum spin Hall insulator to zero gap semimetal to trivial insulator

Buckled Honeycomb Layers: Electric Field Tunable Topology



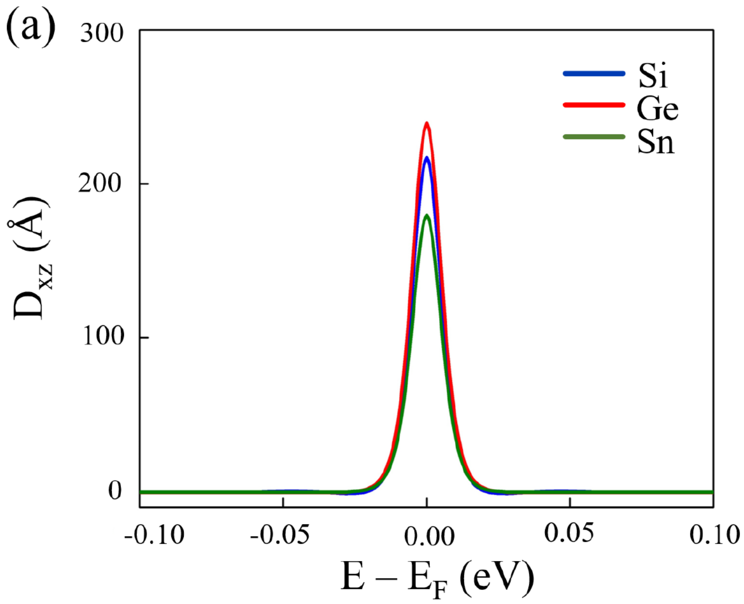
- Phase diagram of strained system similar to pristine case
- Focus near electric field critical value E_c

Buckled Honeycomb Layers: Electric Field Tunable Berry Curvature



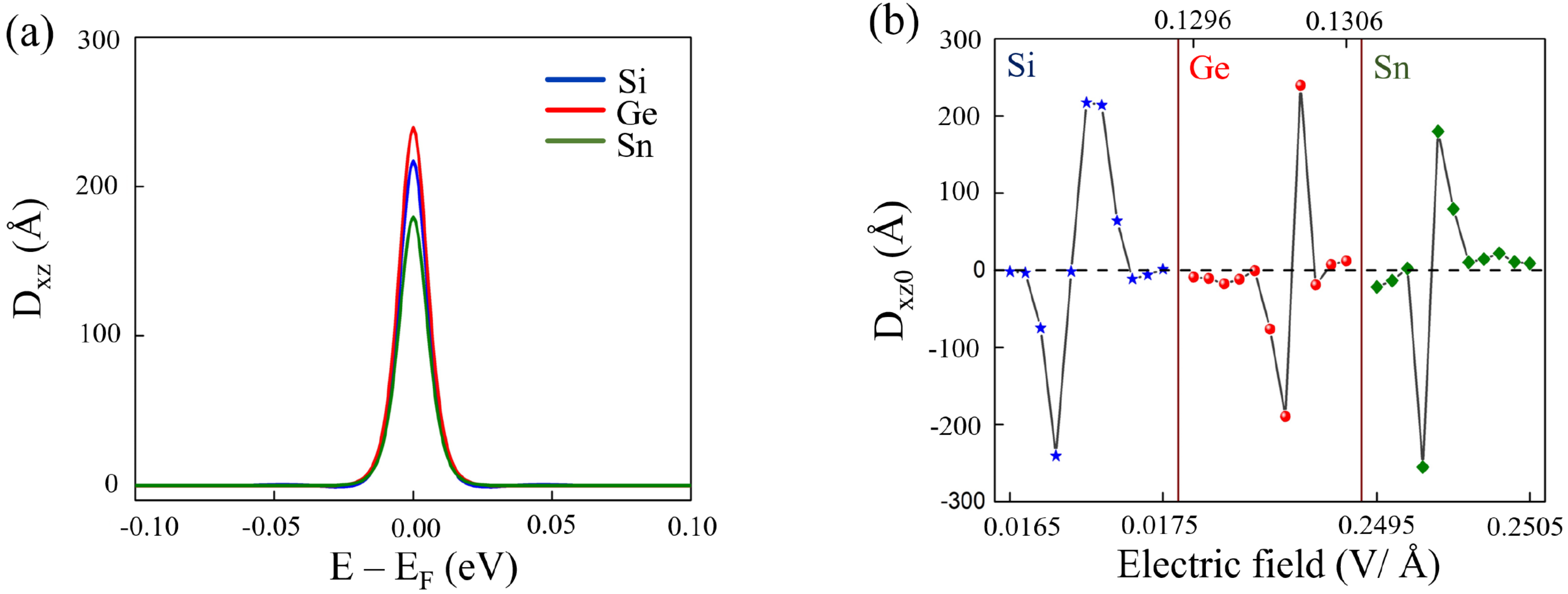
- Berry curvature flips sign across the topological phase transition
- Indicates interesting Berry curvature dipole physics

Buckled Honeycomb Layers: Electric Field Tunable Berry Curvature Dipole



- Giant peak in BCD around Fermi level near critical electric fields
- Enhanced BCD a signature of topological to trivial insulator transition

Buckled Honeycomb Layers: Electric Field Tunable Berry Curvature Dipole



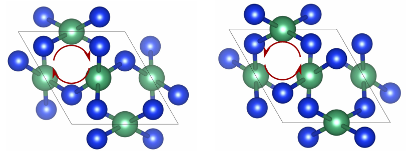
- Giant peak in BCD around Fermi level near critical electric fields
- Enhanced BCD a signature of topological to trivial insulator transition
- Sign of BCD flipped on either side of topological phase transition
- Values highest among untwisted two-dimensional materials

Plan for this talk

Graphene analogs: Silicene, Germanene and Stanene

Bandyopadhyay, Joseph, and Narayan, 2D Materials 9, 035013 (2022)

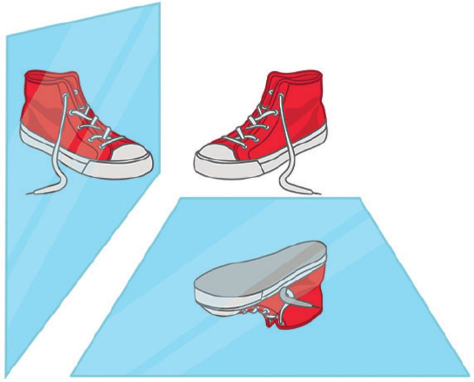
Chiral Materials: Metals, semimetals and semiconductors



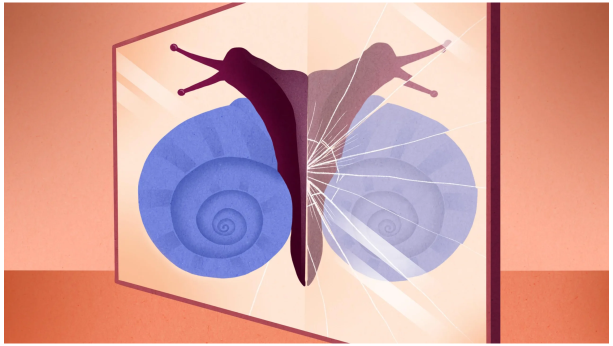
Joseph, Bandyopadhyay, and Narayan, Chemistry of Materials, in press (2024)

Chirality: A brief Introduction

Term first used by Kelvin (1893): "*I call any geometrical figure, or group of points, 'chiral', and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself.*"



Fecher *et al.*, Materials 15, 5812 (2022)



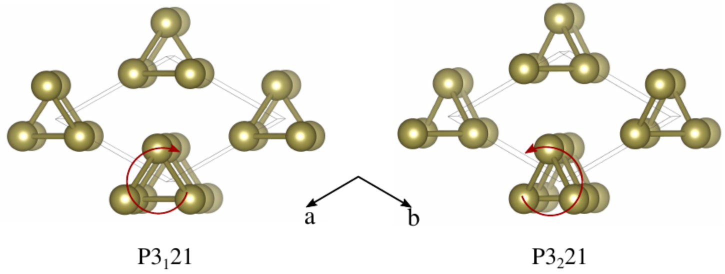
Quanta Magazine: *Magnetism May Have Given Life Its Molecular Asymmetry* (2023)

- Concept of chirality widespread across physics, chemistry, biology...

Chiral Crystals

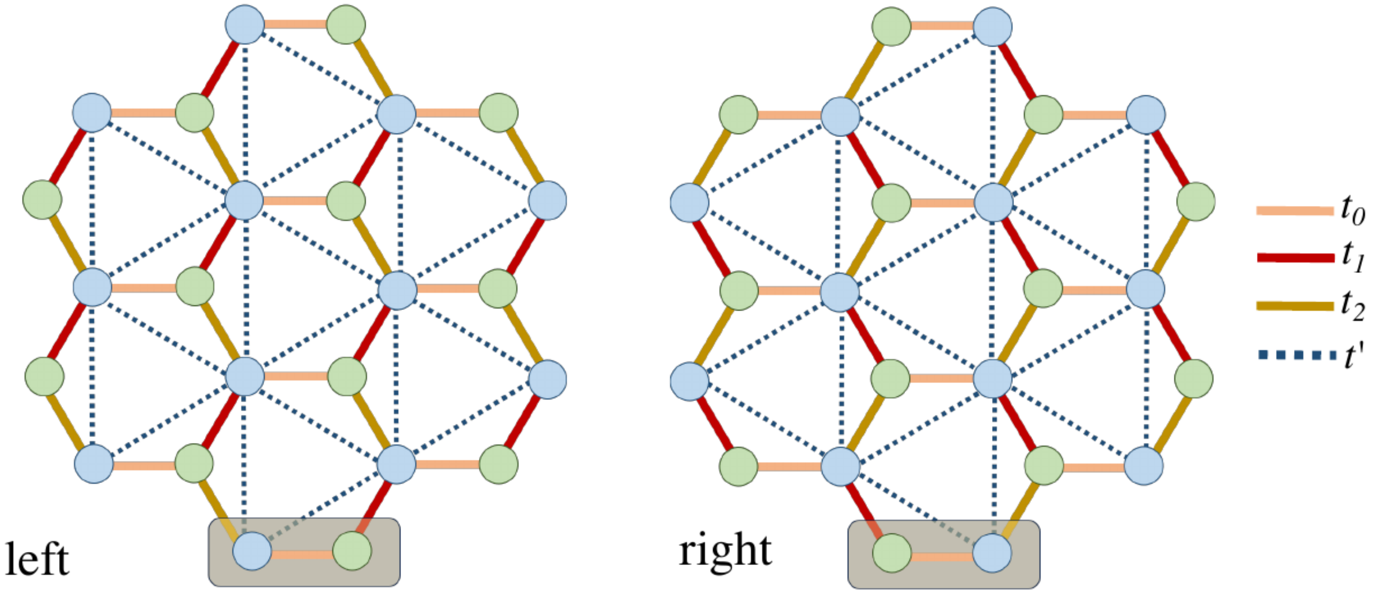
A crystal structure is chiral if its space group consists of only proper operations -- rotations and translations

Elemental Tellurium



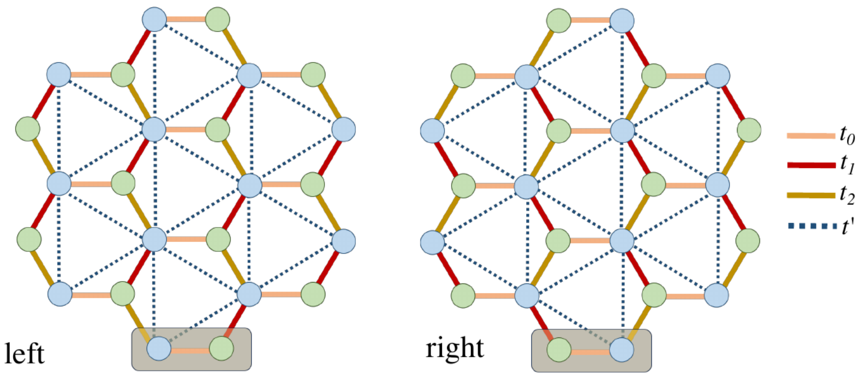
- Inversion, mirror plane, roto-inversion and glide are improper operations
- A number of intriguing aspects of chiral materials have been discovered: interplay with topology, phonons, ferroelectricity
- Non-linear Hall effects?

Chiral Crystals: A simple model



- Honeycomb model inspired by graphene and DNA
- Adjacent hopping parameters are unequal
- Next-nearest neighbour hopping has a handedness – results in chirality

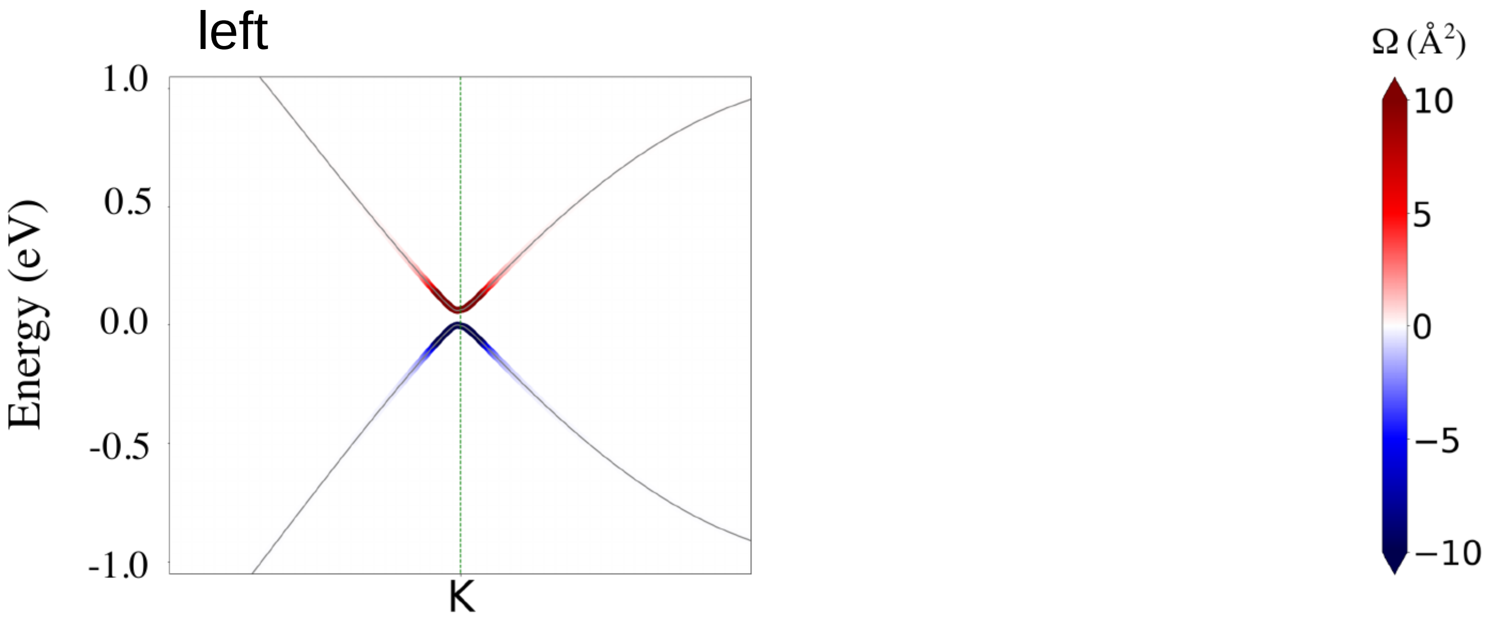
Chiral Crystals: A simple model



$$H = \sum_{\langle i,j \rangle} [t_{ij}\, a_i^\dagger b_j + h.c.] + \sum_{\langle\langle i,j \rangle\rangle} [g_{ij}^l\, a_i^\dagger a_j + g_{ij}^r\, b_i^\dagger b_j + h.c.].$$

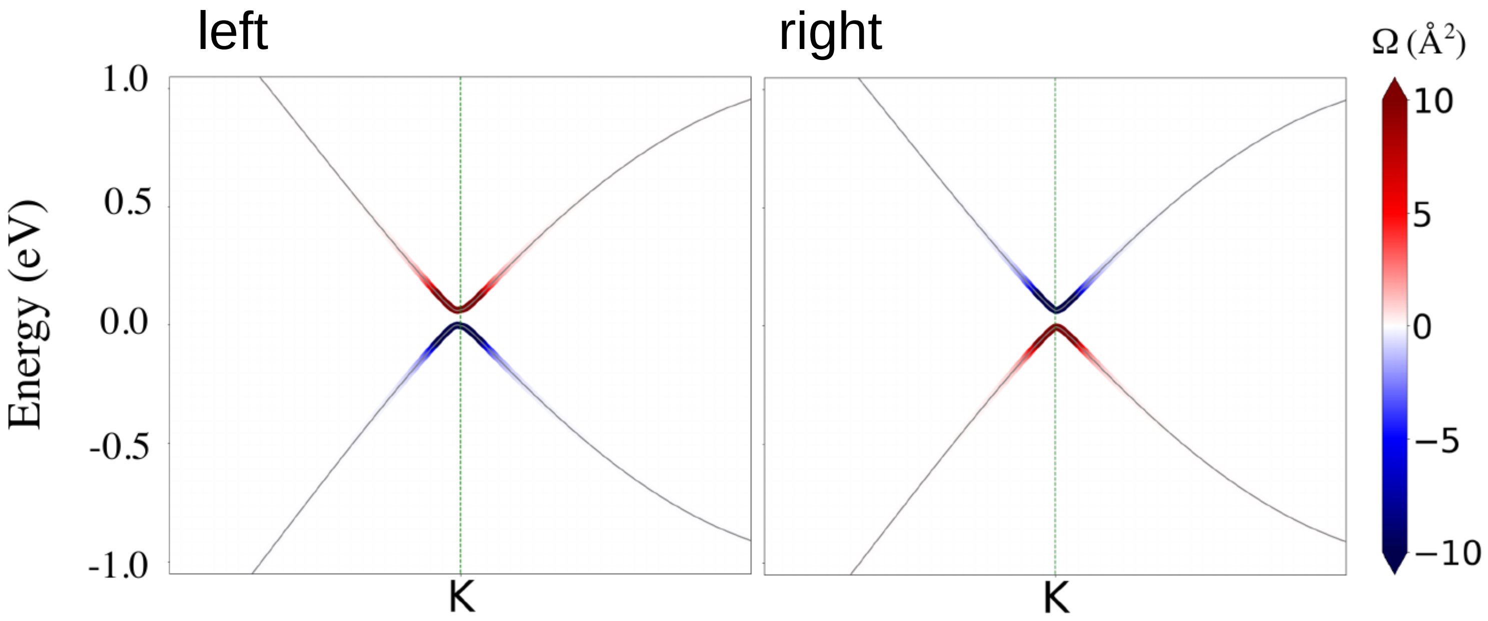
- g^l zero for right-handed structure, g^r zero for left-handed one
- Broken inversion symmetry

Simple model: Berry curvature



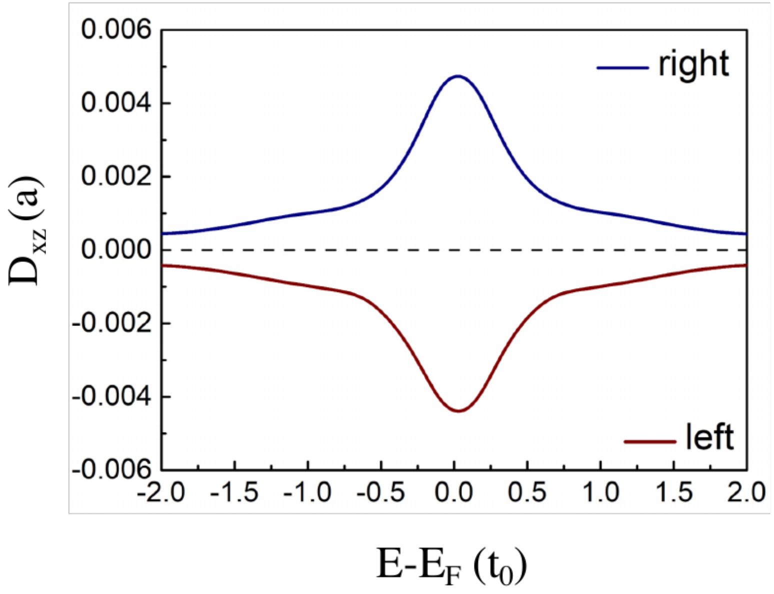
- Broken inversion gives a non-zero Berry curvature
- Concentrated near the band edges as expected

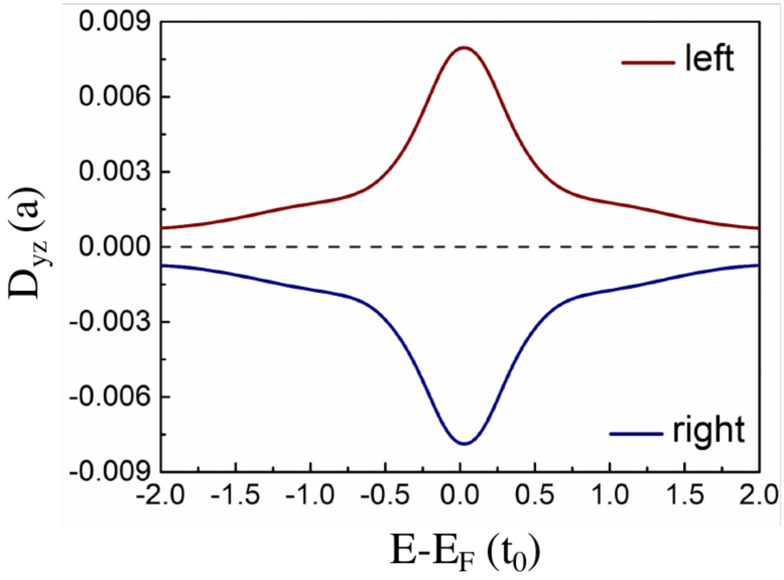
Simple model: Berry curvature



- Broken inversion gives a non-zero Berry curvature
- Concentrated near the band edges as expected
- Right-handed structure has an exactly opposite Berry curvature

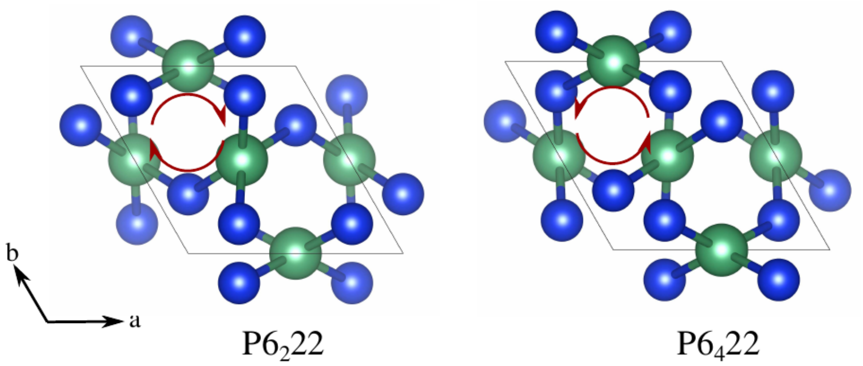
Simple model: Berry curvature dipole

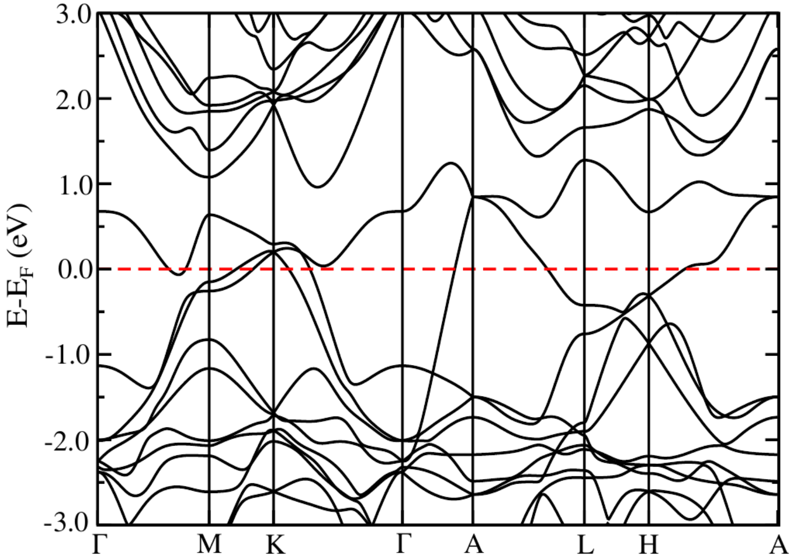




- Two non-zero components of BCD – D_{xz} and D_{yz}
- Right- and left-handed structures give an exactly opposite value of BCD component
- What about real materials?

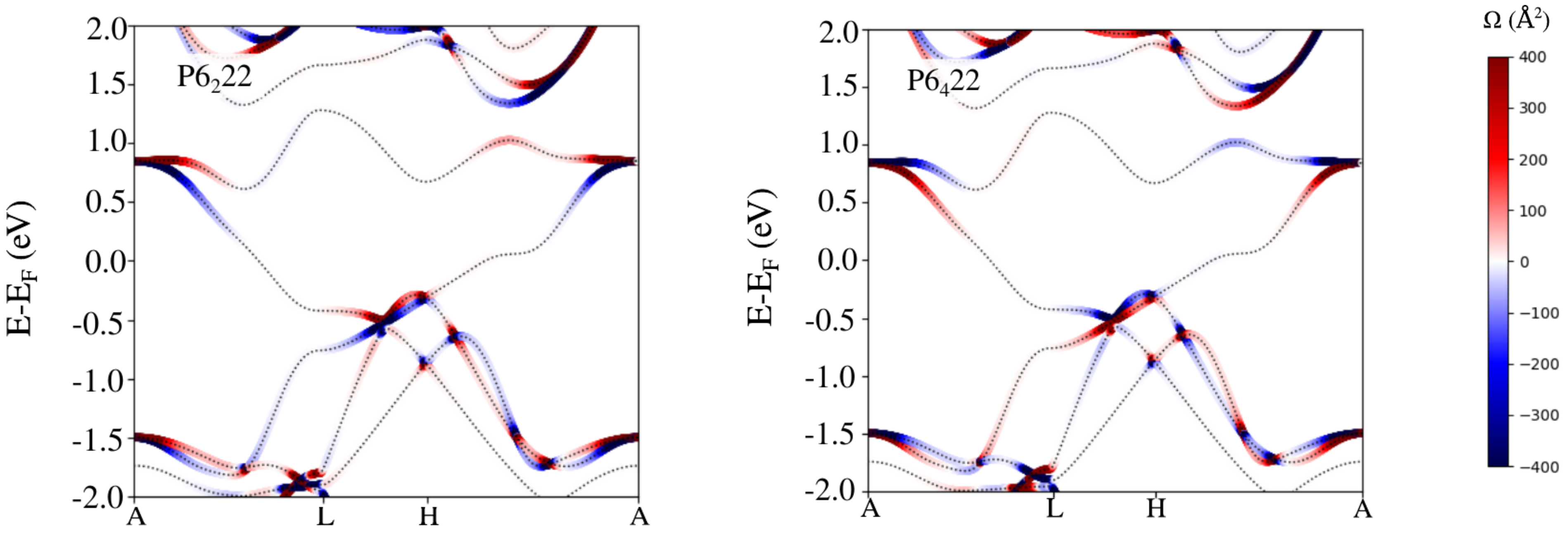
$NbSi_2$: A chiral metal





- Crystallizes in enantiomeric pairs – opposite orientations of Nb-Si-Nb chains
- Metallic with predominantly Nb *d* orbital contribution near Fermi level
- Identical band structure of two enantiomers

$NbSi_2$: Berry curvature



- Berry curvature components have opposite signs for two enantiomers
- A number of Berry curvature hotspots slightly away from Fermi level

$NbSi_2$: Berry curvature dipole tensor symmetries

- Crystal point symmetries impose constraints on the BCD tensor

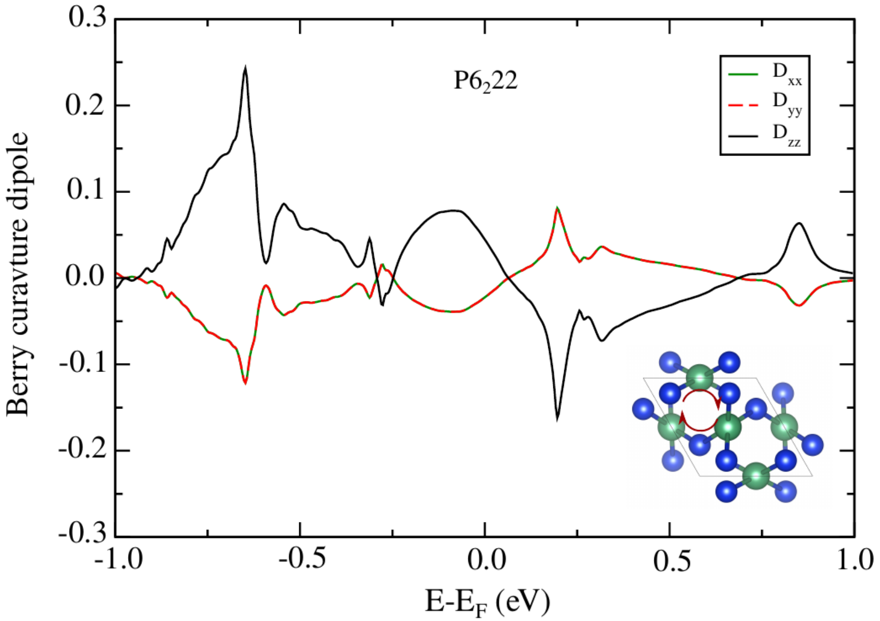
$$D = \det(S) S D S^T$$

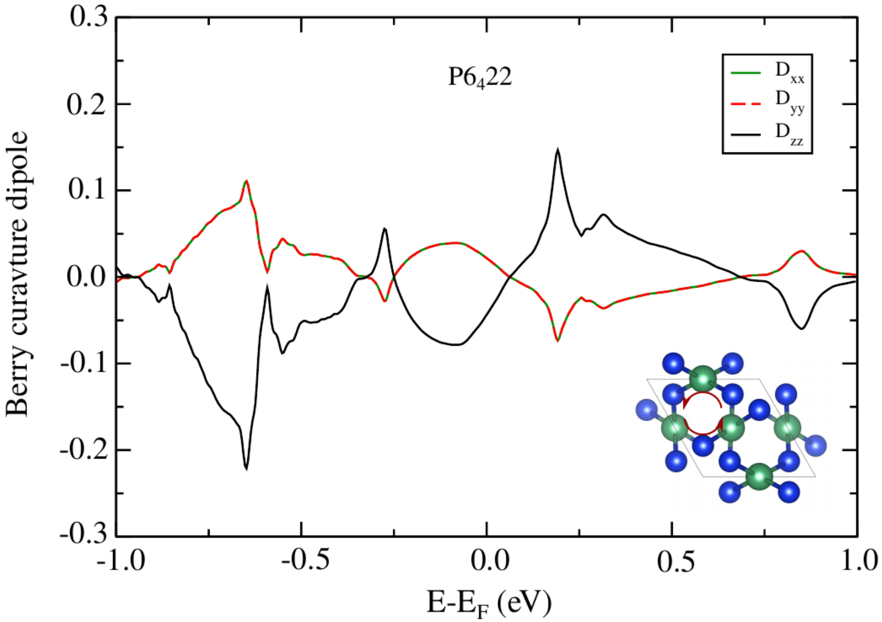
- For $NbSi_2$, one finds the form

$$D = \pm D_{xx} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

- Off-diagonal elements vanish

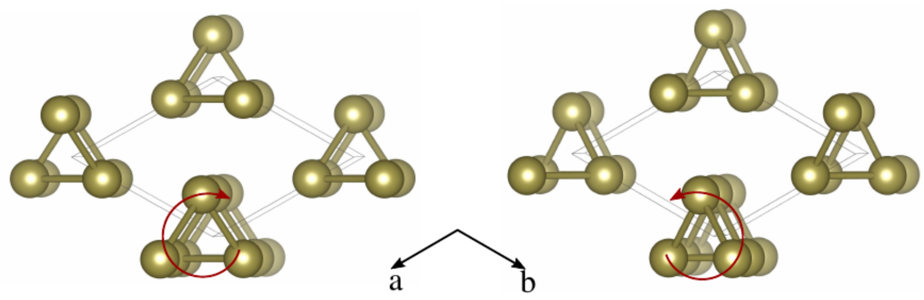
$NbSi_2$: Berry curvature dipole



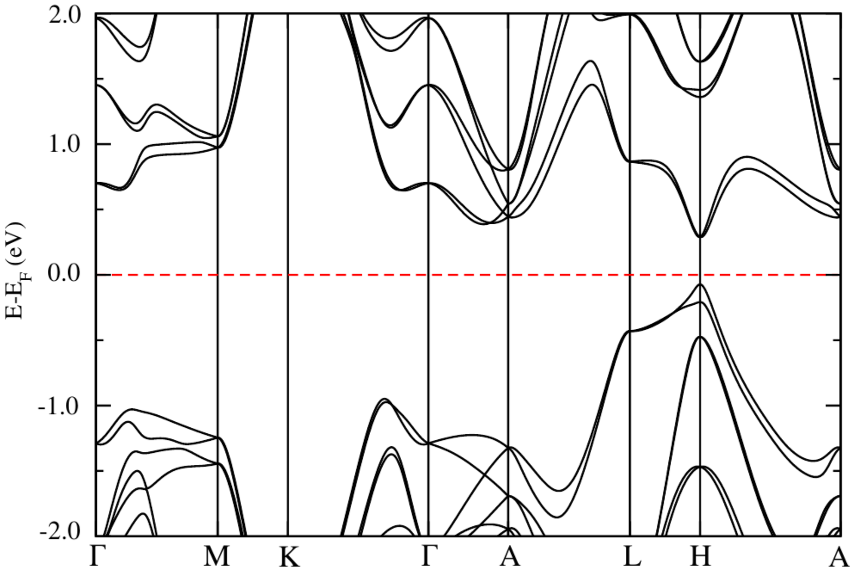


- All components of BCD have opposite signs for two enantiomers
- Peaks occur due to rapidly varying Berry curvature
- Values at Fermi level slightly smaller than TMDCs
- Non-Linear Hall effect – a way to distinguish enantiomeric pairs?

Trigonal Te: An elemental chiral material

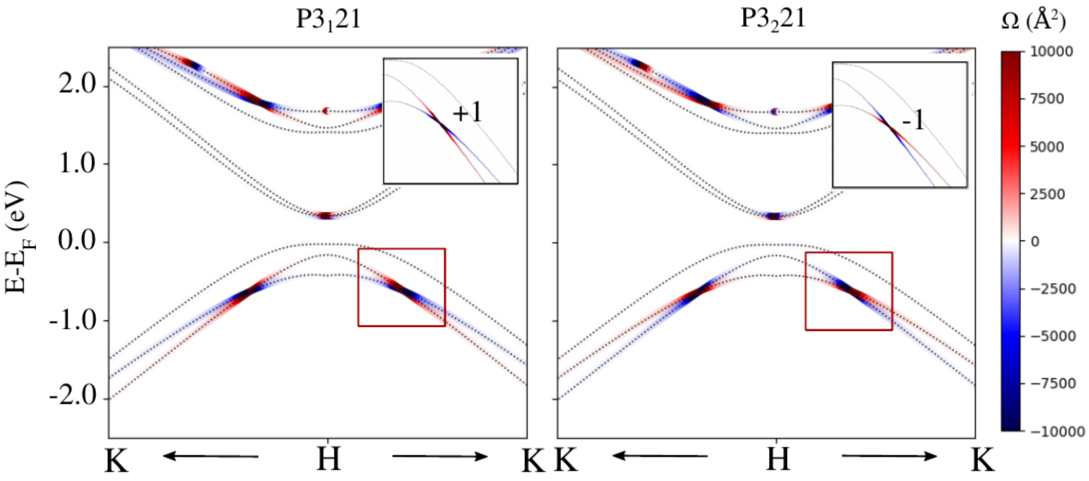


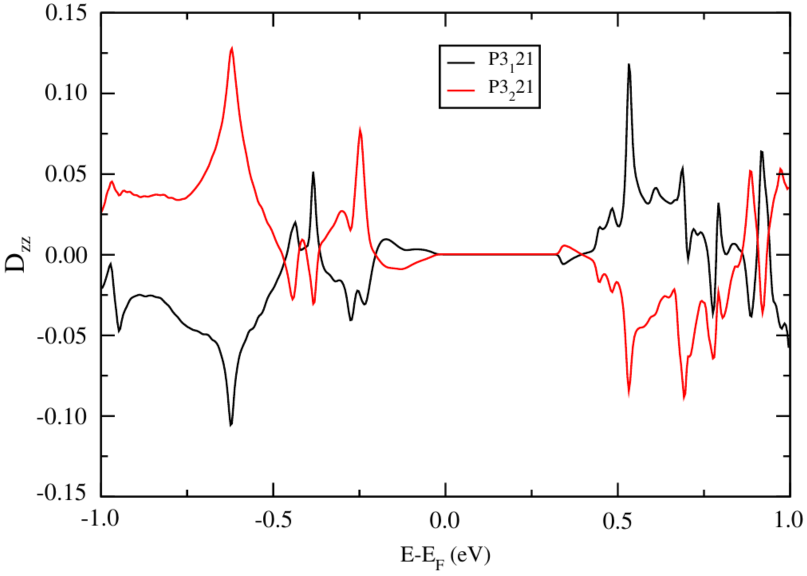
$P3_121$ $P3_221$



- “Hydrogen atom” of chiral materials
- Narrow band gap with topological band crossings in valence and conduction manifolds
- Need hybrid DFT for accurate band structure

Trigonal Te: Berry curvature and dipole

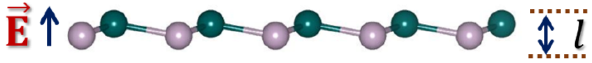




- Opposite Berry curvature for two enantiomers
- Weyl points with topological charge – also opposite in two enantiomers
- BCD components change sign for the enantiomers

Summary

Graphene analogs: Silicene, Germanene and Stanene



Bandyopadhyay, Joseph, and Narayan, 2D Materials 9, 035013 (2022)

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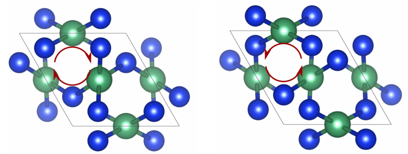

Joseph, Bandyopadhyay, and Narayan, Chemistry of Materials, in press (2024)

Review: Bandyopadhyay, Joseph, and Narayan, Materials Today Electronics 8, 100101 (2024)