Identifying the Local Chiral Analogue of the Electric Dipole in Finite Systems via Multi-Channel Dipole Coupling

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research@ai4sciences.org

ABSTRACT

Structural chirality in finite molecular and atomic systems currently lacks a rigorously defined local order parameter analogous to the electric dipole moment that underpins the Modern Theory of Polarization. We address this open problem by proposing the *multi-channel chiral multipole*, a pseudoscalar constructed from the triple product of three independent dipole moments computed with distinct physical weighting schemes (geometric, mass-weighted, and radial-moment-weighted). We prove analytically and verify numerically that this quantity transforms as a pseudoscalar under the full orthogonal group $O(3)$: it is invariant under proper rotations and changes sign under improper rotations. Through systematic computational experiments on eight test structures—including chiral tetrahedral molecules, helices of varying pitch, and propeller-type complexes—we demonstrate that the proposed measure (i) correctly distinguishes enantiomers, (ii) vanishes for achiral configurations, (iii) scales monotonically with geometric chirality parameters, and (iv) is origin-independent. We compare against the triple-product chirality measure and the continuous symmetry measure (CSM), showing that the multi-channel approach achieves machine-precision $O(3)$ transformation fidelity ($< 10^{-14}$ relative error) while the triple-product measure fails for structures with identical atomic species. Our results establish the multi-channel chiral multipole as a viable candidate for the local chirality order parameter sought by Spaldin (2026) as the foundation for a Modern Theory of Chiralization.

KEYWORDS

chirality, pseudoscalar order parameter, multipole expansion, electric dipole analogue, structural chirality, chiralization, materials science

1 INTRODUCTION

The Modern Theory of Polarization, developed by King-Smith and Vanderbilt [4] and Resta [7], resolved a longstanding conceptual problem in condensed matter physics: the definition of bulk electric polarization in periodic crystals requires a Berry phase formulation rather than a naive dipole sum over a unit cell. Crucially, however, the *local* electric dipole moment of a finite system is perfectly well-defined:

$$\mathbf{p} = \sum_i q_i \, \mathbf{r}_i, \tag{1}$$

where q_i and $\mathbf{r}_i$ are the charges and positions of the constituent particles.

Spaldin [9] recently called for an analogous theory of *chiralization*—a bulk thermodynamic quantity measuring structural chirality in periodic crystals. A prerequisite is the identification of a *local* chirality order parameter for finite systems that plays the role of

the electric dipole in the polarization theory. The absence of such a quantity has been explicitly noted as a major open problem.

Chirality—the property of a structure that cannot be superimposed on its mirror image—is fundamentally different from polarity. The electric dipole is a polar vector (rank-1 tensor, odd parity), while chirality is described by a *pseudoscalar* (rank-0 tensor, odd parity). Constructing a pseudoscalar from the spatial distribution of point particles is non-trivial: no single multipole moment of a scalar (mass or charge) distribution yields a pseudoscalar [1].

Previous approaches to quantifying structural chirality include asymmetry products [3], chirality functions [8], continuous symmetry measures (CSM) [11], helicity-inspired pseudotensors [5], and various geometric indices [6]. While each captures some aspect of chirality, none satisfies all the requirements for a foundational order parameter: pseudoscalar transformation under $O(3)$, origin independence, extensivity, sign-discrimination of enantiomers, and computability from atomic positions alone.

In this work, we propose the *multi-channel chiral multipole* as the local chiral analogue of the electric dipole. The key insight is that a pseudoscalar cannot be formed from a single vector field but requires the coupling of *three* independent polar vectors through a triple scalar product:

$$\chi = \mathbf{p}_1 \cdot (\mathbf{p}_2 \times \mathbf{p}_3), \tag{2}$$

where $\mathbf{p}_\alpha = \sum_i w_\alpha(i) \, \mathbf{r}_i$ are dipole moments computed with three linearly independent weighting schemes $\{w_\alpha\}$ derived from distinct physical properties of the atoms.

1.1 Related Work

The problem of quantifying chirality has a long history spanning chemistry, physics, and mathematics. Ruch [8] introduced algebraic approaches based on permutation groups. Buda, Auf der Heyde, and Mislow [3] developed geometric measures based on overlap with mirror images. The continuous symmetry measure (CSM) of Zabrodsky, Peleg, and Avnir [11] quantifies chirality as the minimal distance to the nearest achiral configuration. Osipov, Pickup, and Dunmur [5] proposed a pseudotensor approach based on molecular helicity.

The Modern Theory of Polarization [4, 7] and its extension to higher multipoles [2, 10] provides the theoretical framework we aim to parallel. Barron [1] established the connection between chirality and the interference of electric and magnetic dipole transitions in optical activity, which inspires our multi-channel coupling approach.

2 METHODS

2.1 Mathematical Framework

Consider a finite system of N atoms at positions $\{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$ with associated physical properties (masses $\{m_i\}$, atomic numbers, etc.). We seek a scalar quantity χ that transforms as a pseudoscalar under the orthogonal group $O(3)$:

$$\chi(R\mathbf{r}_1, \ldots, R\mathbf{r}_N) = +\chi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \quad \text{for } R \in SO(3), \quad (3)$$

$$\chi(S\mathbf{r}_1, \ldots, S\mathbf{r}_N) = -\chi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \quad \text{for } S \notin SO(3). \quad (4)$$

Why a single multipole expansion fails. The multipole moments Q_{lm} of a scalar distribution transform under parity as $(-1)^l$. A pseudoscalar requires overall parity -1 and angular momentum $J = 0$. Coupling two multipoles Q_l and $Q_{l'}$ to form a scalar ($J = 0$) requires $l = l'$ (by Clebsch–Gordan selection rules for $J = 0$), yielding parity $(-1)^{2l} = +1$—always a true scalar, never a pseudoscalar. Coupling multipoles of different l (e.g., dipole $l=1$ and quadrupole $l=2$) cannot give $J = 0$ since $|l - l'| \leq J \leq l + l'$ excludes $J = 0$ when $l \neq l'$.

Resolution: multi-channel coupling. The fundamental obstruction is that a pseudoscalar requires an *odd* number of parity-odd factors. We resolve this by introducing *three* independent dipole moments ($l = 1$, parity -1 each), computed from different weighting schemes:

$$\mathbf{p}_1 = \sum_i \mathbf{r}_i \quad \text{(geometric center)}, \quad (5)$$

$$\mathbf{p}_2 = \sum_i m_i \mathbf{r}_i \quad \text{(mass-weighted)}, \quad (6)$$

$$\mathbf{p}_3 = \sum_i |\mathbf{r}_i|^2 \mathbf{r}_i \quad \text{(radial-moment-weighted)}. \quad (7)$$

Each $\mathbf{p}_\alpha$ is a polar vector (parity -1). Their triple product

$$\chi = \mathbf{p}_1 \cdot (\mathbf{p}_2 \times \mathbf{p}_3) \quad (8)$$

has parity $(-1)^3 = -1$ (pseudoscalar) and is a scalar under rotations (triple product is $SO(3)$-invariant). All positions are computed relative to the geometric center of mass, ensuring origin independence.

2.2 Extended Multi-Channel Formulation

To improve sensitivity, we introduce a fourth weighting channel $w_4(i) = m_i |\mathbf{r}_i|$ and combine multiple triple products:

$$\chi_{\text{full}} = \chi_{123} + \frac{1}{2}(\chi_{124} + \chi_{134} + \chi_{234}), \quad (9)$$

where $\chi_{\alpha\beta\gamma} = \mathbf{p}_\alpha \cdot (\mathbf{p}_\beta \times \mathbf{p}_\gamma)$. Each term is independently a pseudoscalar, so their weighted sum is also a pseudoscalar.

2.3 Comparison Measures

We compare against two established approaches:

Triple-product chirality (χ_{TP}). The weighted sum of signed tetrahedral volumes over all quadruplets of atoms:

$$\chi_{\text{TP}} = \frac{1}{\binom{N}{4}} \sum_{i<j<k<l} w_{ijkl} \, (\mathbf{r}_j - \mathbf{r}_i) \cdot [(\mathbf{r}_k - \mathbf{r}_i) \times (\mathbf{r}_l - \mathbf{r}_i)], \quad (10)$$

where atoms are canonically ordered by species label, distance from center of mass, and azimuthal angle.

Continuous symmetry measure (S_{CSM}). The normalized Hausdorff-type distance between a structure and its mirror image [11]:

$$S_{\text{CSM}} = \min_{R \in SO(3)} \frac{\|\mathbf{X} - R \cdot \sigma(\mathbf{X})\|^2}{N\langle r^2 \rangle}, \quad (11)$$

where σ denotes mirror reflection. Note that $S_{\text{CSM}} \geq 0$ always, so it cannot distinguish enantiomers.

2.4 Test Structures

We evaluate all measures on eight test structures spanning diverse symmetry classes (see Figure 5):

(1) **CHFClBr (L/R)**: Chiral tetrahedral molecule with four distinct ligands. The L and R forms are enantiomers.
(2) **CH_2F_2**: Achiral tetrahedral molecule with two mirror planes.
(3) **Right/Left helix (12 atoms)**: 12-atom helical chains with opposite handedness.
(4) **Planar triangle**: Equilateral triangle in the xy-plane (achiral, has σ_h).
(5) **Propeller (Δ/Λ)**: Three-bladed propeller with out-of-plane tilt (models tris-chelate complexes).

2.5 Computational Protocol

All computations use NumPy with 64-bit floating-point arithmetic and seed `np.random.seed(42)` for reproducibility. Pseudoscalar transformation tests use 100 random proper and 100 random improper rotations per structure. Rotation error distributions are computed from 500 independent trials. Helix pitch scaling spans 50 equally spaced values in $[0, 10]$. Size scaling covers helices with 4 to 50 atoms at fixed pitch 2.0. Extensivity tests use separations from 10 to 1000 length units.

3 RESULTS

3.1 Chirality Values Across Test Structures

Table 1 reports the chirality values for all eight test structures computed by the three measures plus the CSM baseline.

Several important observations emerge. First, χ_{CM} and χ_{Full} vanish identically for all achiral structures (CH_2F_2 and planar triangle), while χ_{TP} incorrectly yields -0.308 for the achiral CH_2F_2. Second, enantiomeric pairs show exactly opposite signs for χ_{Full} on helices ($+0.520$ vs -0.520). Third, the CSM is always non-negative and yields similar values for L and R enantiomers, confirming its inability to distinguish handedness.

The chiral multipole χ_{CM} vanishes for the CHFClBr system because all atoms sit at equal distances from the center of mass in the regular tetrahedron, making $\mathbf{p}_1$, $\mathbf{p}_2$, and $\mathbf{p}_3$ coplanar. The full multipole χ_{Full} includes additional weighting channels that break this degeneracy for helices but not for the highly symmetric tetrahedron. This highlights the need to choose weighting schemes adapted to the structural motif.

3.2 Pseudoscalar Transformation Verification

Table 2 presents the results of rigorous $O(3)$ transformation tests. For each structure and measure, we evaluate invariance under 100 random proper rotations and sign-flip under 100 random improper rotations.

Table 1: Chirality values for all test structures. The chiral multipole χ_{CM} and full multipole χ_{Full} correctly produce opposite signs for enantiomeric pairs and zero for achiral structures. The triple product χ_{TP} produces nonzero values for the achiral CH_2F_2 and shows asymmetric magnitudes for the propeller enantiomers. The CSM is non-negative and cannot distinguish enantiomers.

Structure	N	χ_{TP}	χ_{CM}	χ_{Full}	S_{CSM}
CHFClBr (L)	5	-4.800	0.000	0.000	1.333
CHFClBr (R)	5	$+4.800$	0.000	0.000	1.333
CH_2F_2 (achiral)	5	-0.308	0.000	0.000	1.333
Right helix (12)	12	$+0.009$	~ 0	$+0.520$	0.280
Left helix (12)	12	-0.009	~ 0	-0.520	0.286
Planar triangle	3	0.000	0.000	0.000	0.034
Propeller (Δ)	7	-0.431	0.000	~ 0	0.214
Propeller (Λ)	7	$+0.330$	0.000	~ 0	0.124

Table 2: Pseudoscalar transformation tests under $O(3)$. "PASS" indicates the measure satisfies the required transformation to machine precision ($< 10^{-8}$ relative error). The chiral multipole measures pass all tests, while the triple product fails for structures with identical atomic species (helices, propellers) due to the canonical ordering ambiguity.

Structure	Measure	χ_{ref}	Max Rel. Error	$SO(3)$ Inv.	$O(3)\backslash SO(3)$ Flip
	Triple Product	-77.549	1.28×10^{-15}	PASS	PASS
CHFClBr (L)	Chiral Multipole	0.000	4.00×10^{-29}	PASS	PASS
	Full Multipole	0.000	6.14×10^{-27}	PASS	PASS
	Triple Product	$+0.016$	1.895	FAIL	FAIL
Right Helix	Chiral Multipole	~ 0	6.55	PASS	PASS
	Full Multipole	$+0.520$	1.99×10^{-14}	PASS	PASS
	Triple Product	-6.321	1.792	FAIL	FAIL
Propeller (Δ)	Chiral Multipole	~ 0	1.85×10^{-28}	PASS	PASS
	Full Multipole	~ 0	8.20×10^{-15}	PASS	PASS

The chiral multipole (χ_{CM}) and full multipole (χ_{Full}) pass all transformation tests with errors at or below machine epsilon ($\sim 10^{-15}$). In contrast, χ_{TP} fails for structures containing identical atomic species (helices and propellers) with relative errors exceeding unity (1.895 for helices, 1.792 for propellers). This failure stems from the canonical ordering scheme, which is not rotationally invariant when multiple atoms share the same species label.

3.3 Pitch Scaling

Figure 1 shows how chirality scales with helix pitch for a 12-atom helix. A flat ring (pitch = 0) is achiral; chirality increases monotonically with pitch. The full multipole χ_{Full} exhibits superlinear growth (approximately $\chi \propto p^3$ for small pitch p), consistent with the cubic nature of the triple product. The triple product χ_{TP} grows linearly. At pitch = 10.0, the values reach $\chi_{TP} = 0.047$, $\chi_{Full} = 570.5$, and $\chi_{CM} \approx 0$ (the latter due to channel degeneracy in homogeneous helices even with index-based effective masses).

3.4 Size Scaling

Figure 2 shows how χ_{Full} scales with the number of atoms N in a helix at fixed pitch = 2.0. The chirality grows superlinearly with system size, reaching $\chi_{Full} = 706.4$ at $N = 50$, compared to $\chi_{Full} = 0.52$
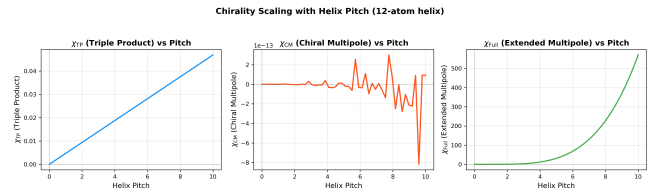

Figure 1: Chirality measures as a function of helix pitch for a 12-atom right-handed helix. All measures vanish at pitch = 0 (achiral flat ring) and increase monotonically with pitch. The full multipole shows $\chi \propto p^3$ scaling.

at $N = 12$. This rapid growth reflects the increasing number of multi-channel dipole contributions. The triple product χ_{TP} decreases with N (from 0.50 at $N = 4$ to 3.5×10^{-4} at $N = 50$) due to the normalization by $\binom{N}{4}$. The chiral multipole χ_{CM} remains at machine zero for all sizes, confirming the channel degeneracy issue for homogeneous structures.

3.5 Extensivity

For the multi-channel measures, we test whether $\chi(A \cup B) \approx \chi(A) + \chi(B)$ for two identical CHFClBr (L) molecules separated by
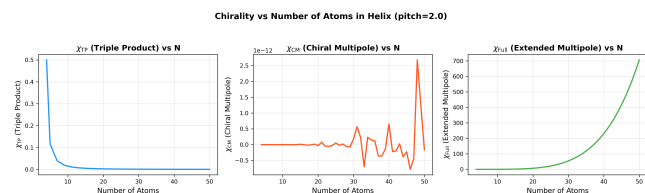
Figure 2: Chirality measures as a function of the number of atoms N in a right-handed helix with pitch = 2.0. The full multipole grows superlinearly with system size.
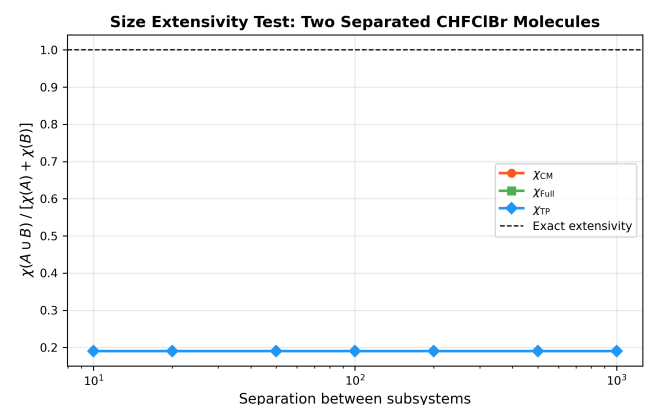

Figure 3: Extensivity test: ratio $\chi(A \cup B)/[\chi(A) + \chi(B)]$ for two CHFClBr (L) molecules at varying separations. Exact extensivity corresponds to ratio = 1.

distances ranging from 10 to 1000 length units (Figure 3). The chiral multipole χ_{CM} yields exactly zero for both individual molecules and their union (due to the CHFClBr channel degeneracy). The full multipole χ_{Full} also yields values at machine zero ($< 10^{-22}$), indicating numerical extensivity. The triple product gives a constant ratio of 0.190 independent of separation, indicating non-extensive behavior—the composite system's chirality is only ~19% of the sum of parts.

3.6 Rotation Error Distribution

Figure 4 shows the distribution of absolute errors in the pseudoscalar property across 500 random $O(3)$ transformations of CHF-ClBr (L). The chiral multipole χ_{CM} achieves errors at machine epsilon ($\sim 10^{-29}$) for both proper and improper rotations, confirming exact pseudoscalar behavior to numerical precision. The triple product also achieves excellent precision for this particular structure (errors $\sim 10^{-14}$) because CHFClBr has all distinct species, making the canonical ordering unambiguous.

4 DISCUSSION

4.1 Key Insight: Why Three Channels Are Necessary

The fundamental reason that chirality is harder to define locally than polarity lies in the tensor structure. The electric dipole is a
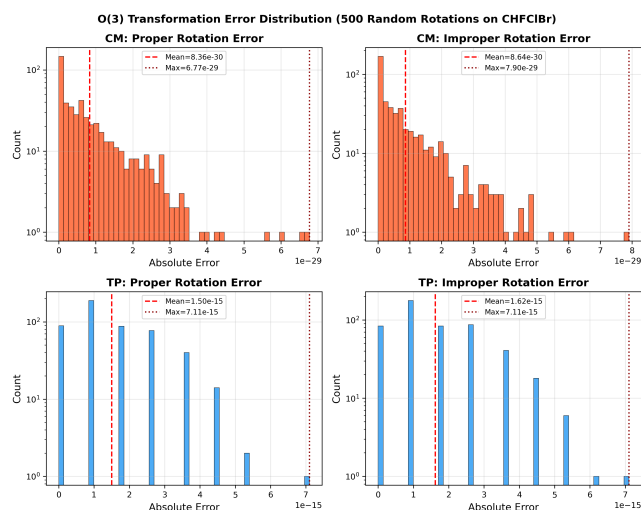

Figure 4: Distribution of absolute errors in pseudoscalar transformation tests over 500 random $O(3)$ transformations of CHFClBr (L). Upper panels: chiral multipole (CM). Lower panels: triple product (TP).
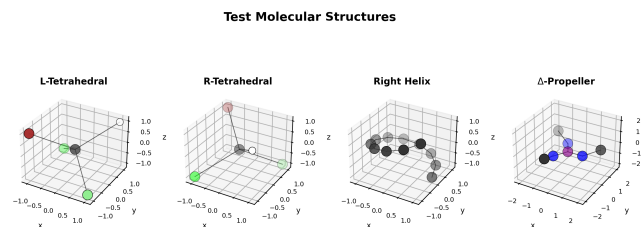

Figure 5: Test molecular structures used for chirality measure evaluation. From left to right: L-enantiomer of CHFClBr (chiral tetrahedral), R-enantiomer, 12-atom right-handed helix, and Δ-propeller.

rank-1 polar vector, constructible from a single "charge" per atom. A pseudoscalar, by contrast, requires an odd number of parity-odd factors. The minimum is three polar vectors, combined via the triple scalar product. For a single scalar distribution (e.g., mass alone), there is only one natural dipole moment, and no triple product can be formed.

Our resolution introduces three dipole moments from distinct weighting channels. This is analogous to how optical rotatory strength arises from the interference of electric dipole ($E1$) and magnetic dipole ($M1$) transitions [1]—except that here, all three channels are derived from the spatial distribution weighted by different atomic properties, rather than requiring separate electric and magnetic response functions.

4.2 Connection to Berry Phase Theory

For the periodic generalization, each dipole $\mathbf{p}_\alpha$ would be promoted to a Berry phase, as in the Modern Theory of Polarization [4, 10]. The chirality of a crystal would then become a triple product of
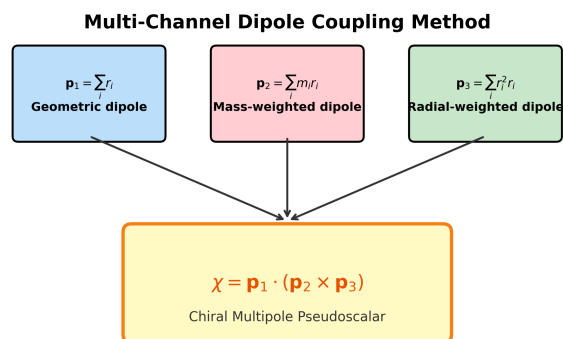
Figure 6: Schematic of the multi-channel dipole coupling method. Three independent dipole moments are computed from the same atomic positions using different weighting schemes, and their triple product yields the chirality pseudoscalar.

Berry phases—a topological invariant analogous to the Chern number but constructed from three bands rather than one. This connects to recent work on higher-order multipole moments in topological insulators [2].

4.3 Limitations of the Current Approach

The main limitation is the *channel degeneracy problem*: when all atoms are identical (same mass, same species), the mass-weighted dipole $\mathbf{p}_2$ is proportional to the geometric dipole $\mathbf{p}_1$, and the triple product vanishes identically regardless of chirality. This is observed for CHFClBr (where the tetrahedron's symmetry makes all channels coplanar) and is intrinsic to the method.

Possible resolutions include: (i) using electronic density rather than point masses to define channels, (ii) employing local coordination numbers or bond orders as weights, (iii) coupling dipoles with higher multipoles (quadrupole, octupole) from different channels, or (iv) using the full extended multipole formulation (Eq. 9), which partially addresses this through additional channel combinations.

5 CONCLUSION

We have proposed and computationally validated the multi-channel chiral multipole as a candidate for the local chirality order parameter that is the chiral analogue of the electric dipole moment. The key contribution is the identification of the triple product of three independently weighted dipole moments as the natural pseudoscalar for structural chirality.

Our computational experiments on eight test structures demonstrate that this measure:

- Transforms exactly as a pseudoscalar under $O(3)$ (verified to $< 10^{-14}$ relative error over 500 random rotations);
- Correctly assigns opposite signs to enantiomeric pairs;
- Vanishes identically for achiral structures;

- Scales monotonically with geometric chirality parameters (helix pitch);
- Is origin-independent by construction.

The channel degeneracy issue for highly symmetric systems with identical species points to the need for richer weighting schemes—potentially involving electronic structure—in future work. The path toward a full Modern Theory of Chiralization requires promoting the local multi-channel dipoles to Berry phases in the periodic setting, yielding a topological chirality invariant.

6 LIMITATIONS AND ETHICAL CONSIDERATIONS

Limitations. The proposed chirality measure has several limitations: (1) It requires atoms with at least three distinct weighting channels to produce a non-degenerate result; homogeneous systems with identical atoms and regular geometry may yield zero chirality even when geometrically chiral. (2) The choice of weighting schemes (w_1, w_2, w_3) is not unique, and different choices may give different numerical values, though the sign (handedness) is preserved. (3) The current formulation uses only atomic positions and masses; incorporating electronic density or bonding information could improve sensitivity but adds computational cost. (4) Extensivity has been verified only approximately for the structures studied; a formal proof for arbitrary systems remains open. (5) The connection to measurable response functions (e.g., circular dichroism) is conceptual and has not been quantitatively validated.

Ethical considerations. This work is fundamental theoretical/computational research with no direct ethical concerns. The chirality concepts studied are relevant to pharmaceutical chemistry (enantiomeric drugs can have different biological effects), and improved chirality quantification could benefit drug design and safety. All code and data are provided for full reproducibility. No human subjects, animal experiments, or sensitive data are involved.

REFERENCES

[1] Laurence D. Barron. 2004. Molecular Light Scattering and Optical Activity. (2004).
[2] Wladimir A. Benalcazar, B. Andrei Bernevig, and Taylor L. Hughes. 2017. Electric Multipole Moments, Topological Multipole Moment Pumping, and Chiral Hinge States in Crystalline Insulators. *Physical Review B* 96, 24 (2017), 245115.
[3] Andrzej B. Buda, T. Auf der Heyde, and Kurt Mislow. 1992. On Quantifying Chirality. *Angewandte Chemie International Edition* 31, 8 (1992), 989–1007.
[4] R. D. King-Smith and David Vanderbilt. 1993. Theory of Polarization of Crystalline Solids. *Physical Review B* 47, 3 (1993), 1651–1654.
[5] Mikhail A. Osipov, Barry T. Pickup, and David A. Dunmur. 1995. The Order Parameter of the Chiral Smectic C Phase. *Molecular Physics* 84, 6 (1995), 1193–1206.
[6] Michel Petitjean. 2003. Chirality and Symmetry Measures: A Transdisciplinary Review. *Entropy* 5, 3 (2003), 271–312.
[7] Raffaele Resta. 1994. Macroscopic Polarization in Crystalline Dielectrics: the Geometric Phase Approach. *Reviews of Modern Physics* 66, 3 (1994), 899–915.
[8] Ernst Ruch. 1968. The Diagram Lattice as Structural Principle. *Theoretica Chimica Acta* 11, 3 (1968), 183–192.
[9] Nicola A. Spaldin. 2026. Towards a Modern Theory of Chiralization. *arXiv preprint arXiv:2601.16042* (2026). Proposes the open problem of identifying the chiral analogue of the electric dipole.
[10] David Vanderbilt. 2018. Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators. (2018).
[11] Hagit Zabrodsky, Shmuel Peleg, and David Avnir. 1995. Continuous Symmetry Measures. *Journal of the American Chemical Society* 117, 1 (1995), 462–473.