Chiral Population Analysis

Scientific Achievement

In this work, a CINT User Team partitioned circular dichroism signals into atomic orbital contributions to get an accurate and meaningful spatially resolved picture of chirality.

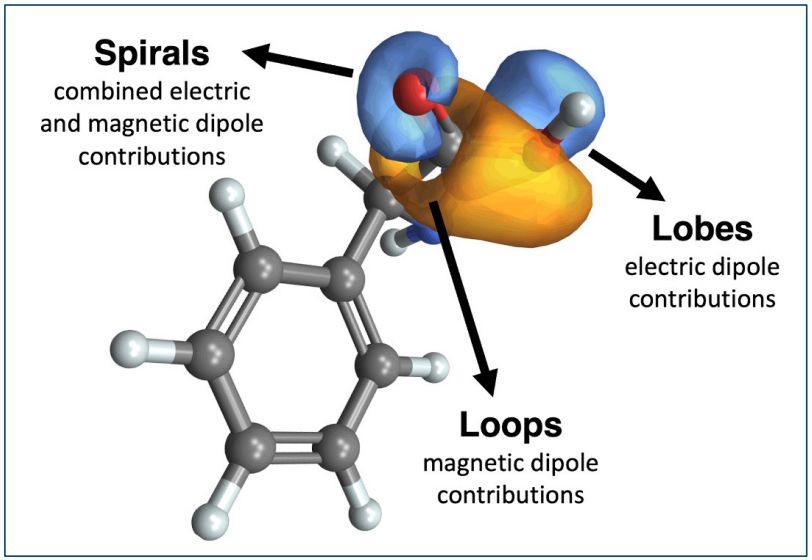

Figure: Chiral Population Analysis (CPA) isosurface plots connects dichroic response to its origins in the atomic orbital picture, allowing the identification of transition dipole induced features, such as spiral motives where both electric and magnetic contributions are relevant.

Significance and Impact

Chiral Population Analysis (CPA) can guide the optimization of chiral ligands by identifying regions of strong rotatory strength and support the rational design of X-ray chromophores for resonant X-ray circular dichroism experiments, where localized transitions enable site-specific chirality measurements.

Research Details

- CPA is built from transition density matrices and dipole operator integrals in the atomic orbital space, which are commonly calculated by standard quantum chemistry software, making it a widely accessible tool.
- CPA can be directly extended to any range of the electromagnetic spectrum and to transitions between excited states.

Work was performed, in part, at the Center for Integrated Nanotechnologies.

Freixas, V. M.; Rouxel, J. R.; Tretiak, S.; Govind, N.; Mukamel, S. Chiral Population Analysis: A Real Space Visualization of X-Ray Circular Dichroism. *Chemical Science.* 2025.