

Deconstructing Chirality with Site-Specific X-Ray Probes

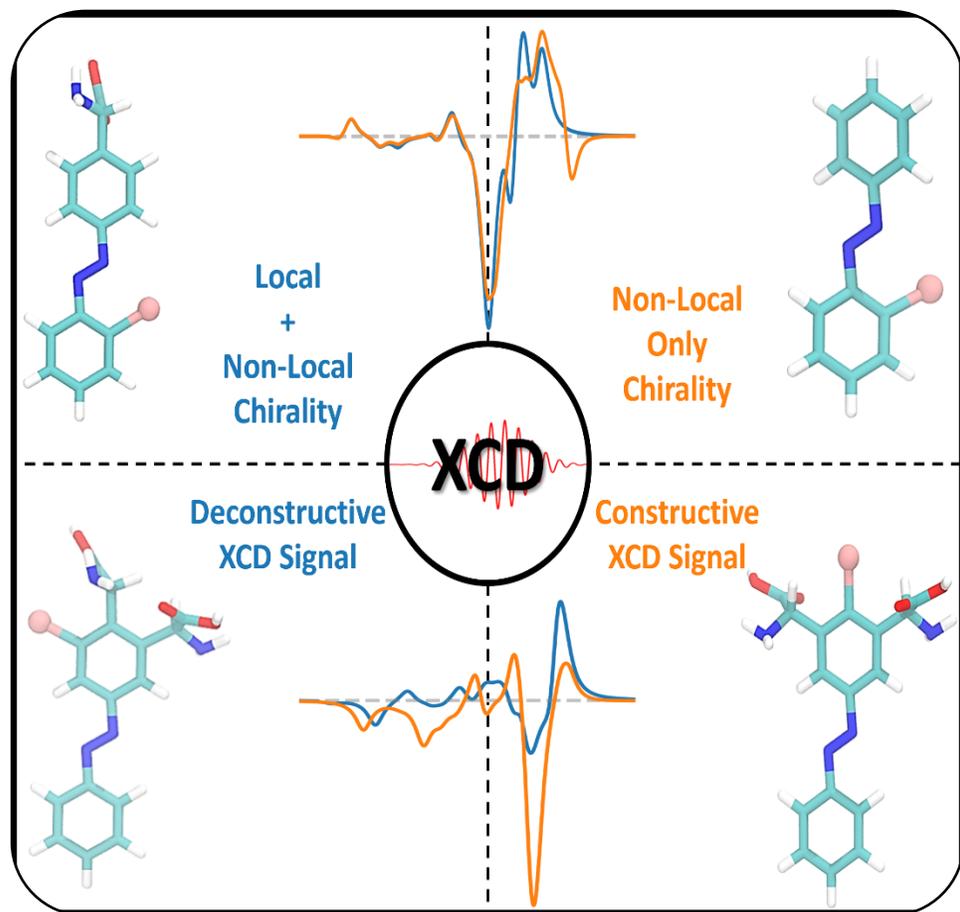


Figure: X-ray Circular Dichroism (XCD) resolves molecular chirality in azobenzene derivatives.

Scientific Achievement

Differentiation of local from non-local chirality revealed that non-local effects can dominate and interfere destructively with local signals. This insight establishes that chiroptical signals can be rationally enhanced through the constructive interference of multiple chiral centers.

Significance and Impact

This work enables the design of novel materials with tailored light-interaction properties and offers a sophisticated framework for interpreting complex CD spectra to precisely identify sources of chirality.

Research Details

- Using Azobenzene, systematically compared Optical CD and X-ray CD responses using quantum chemistry simulations.
- Deconstructed chiroptical signals by varying the positions of the chiral center (glycine) and the X-ray probe (bromine).
- Investigated cooperative steric hindrance between substituents as a method for inducing chiroptical response

Khanna, A.; Freixas, V. M.; Xu, L.; Rouxel, J. R.; Govind, N.; Garavelli, M.; Mukamel, S.; Tretiak, S. Deconstructing Chirality: Probing Local and Nonlocal Effects in Azobenzene Derivatives with X-Ray Circular Dichroism. *The Journal of Physical Chemistry Letters*. 2025.

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