Study provides detailed look at intriguing property of chiral materials

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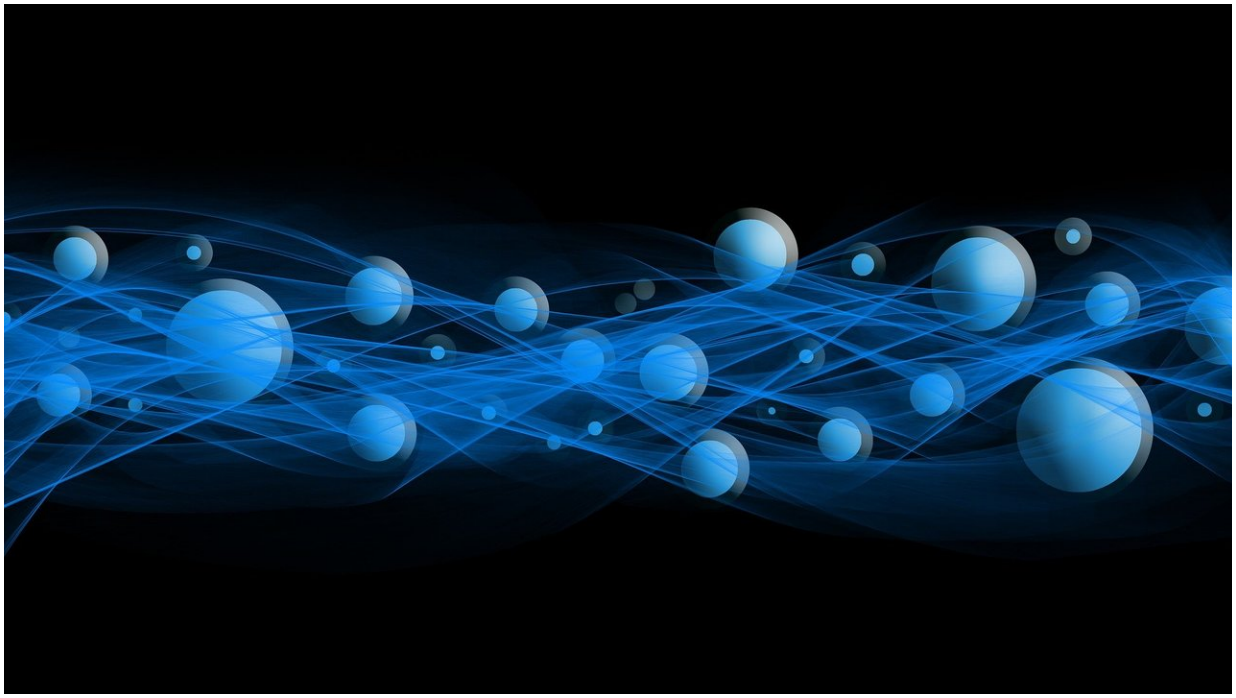

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In nature, many molecules possess a property called chirality, which means that they cannot be superimposed on their mirror images (like a left and right hand).

Chirality can influence function, impacting a pharmaceutical or enzyme's effectiveness, for example, or a compound's perceived aroma.

Now, a new study is advancing scientists' understanding of another property tied to chirality: How light interacts with chiral materials under a magnetic field.

Prior research has shown that in such a system, the left- and right-handed forms of a material absorb light differently, in ways that mirror one another when light flowing parallel to an external magnetic field changes direction, adopting an anti-parallel flow. This phenomenon is called magneto-chiral dichroism (MChD).

Missing, however, from past experiments was a confirmation that experimental observations match up with predictions made by MChD theory—a necessary step in verifying the theory and understanding the effects scientists have observed.

The new paper, which will be published on April 21 in *Science Advances*, changes this. The study was led by Geert L. J. A. Rikken, Ph.D., director of the Laboratoire National des Champs Magnétiques Intenses in France, and Jochen Autschbach, Ph.D., Larkin Professor of Chemistry at the University at Buffalo in the U.S. The first authors were Matteo Atzori, Ph.D., a researcher at the Laboratoire National des Champs Magnétiques Intenses, and UB chemistry Ph.D. student Herbert Ludowieg.

"The first theoretical predictions of MChD for light appeared in 1980s. Since then, an increasing number of observations of the effect have been reported, but no quantitative analysis was possible to confirm whether the underlying theory of MChD is correct," Rikken says. "The new study puts forward detailed measurements on two well-defined model systems, and advanced quantum-chemical calculations on one of them."

"Dr. Rikken's team made the first experimental observation of MChD in 1997 and has since reported other experimental studies of the effect in different systems," Autschbach says. "However, only now has a direct comparison between an experiment and ab-initio quantum theoretical calculations become possible, for a verification of the MChD theory."

The research focused on crystals consisting of the mirrored forms of two compounds: tris(1,2-diaminoethane)nickel(II)nitrate, and tris(1,2-diaminoethane)cobalt(II)nitrate. As Autschbach explains, "the molecular shape of the tris(1,2-diaminoethane)metal(II) ion in the crystal has a propeller-like shape. Propellers come in pairs of mirror images, too, that cannot be superimposed."

Rikken's lab made detailed experimental measurements for both systems studied, while Autschbach's group leveraged UB's supercomputing facility, the Center for Computational Research, to carry out challenging quantum-chemical calculations relating to light absorption by the nickel(II) compound.

The results, as explained in the *Science Advances* paper: "We report the experimental low-temperature MChD spectra of two archetypal chiral paramagnetic crystals taken as model systems, tris(1,2-diaminoethane)nickel(II) and cobalt(II) nitrate, for light propagating parallel or perpendicular to the c-axis of the crystals, and the calculation of the MChD spectra for the Ni(II) derivative by state-of-the-art quantum chemical calculations.

"By incorporating vibronic coupling, we find good agreement between experiment and theory, which opens the way for MChD to develop into a powerful chiral spectroscopic tool and provide fundamental insights for the chemical design of new magnetochiral materials for technological applications."

While the study is in the realm of basic science, Rikken notes the following with regard to the future potential of MChD: "We find experimentally that (for the materials we studied), at low temperatures, the difference in light transmission parallel and anti-parallel to a modest magnetic field of 1 Tesla, hardly more than what a refrigerator magnet produces, can be as high as 10%. Our calculations permit us to understand this in detail. The size of the effect and its detailed understanding now open the door to future applications of MChD, which could range from optical diodes to new optical data storage methods."

More information: Validation of microscopic magnetochiral dichroism theory, *Science Advances* (2021). DOI: 10.1126/sciadv.abg2859 ,
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