Polarized Photoluminescence and Enhanced Circular Dichroism in an Achiral, Low Bandgap Bismuth Iodide Perovskite Derivative

Philip Klement[1], Jakob Möbs[2,3], Gina Stuhrmann[4], Lukas Gümbel[1], Marius J. Müller[1], Johanna Heine[2], and Sangam Chatterjee[1]

[1] *Institute of Experimental Physics I and Center for Materials Research, Justus-Liebig-University Giessen, D-35392 Giessen, Germany*

[2] *Department of Chemistry and Materials Science Center, Philipps-University Marburg, D-35032 Marburg, Germany*

[3] *Present Adress: Department of Physics, University of Oxford, Parks Road, OX1 3PU Oxford, United Kingdom*

[4] *Institute of Nanotechnology (INT) and Karlsruhe Nano Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT), D-76021 Karlsruhe, Germany*

sangam.chatterjee@physik.uni-giessen.de

Lead halide perovskites and related main-group halogenido metalates exhibit unique semiconductor properties, positioning them as promising candidates for next-generation optoelectronics. Their applications span solar cells, light-emitting diodes, lasers, sensors, and photo-catalysis. The approach of assembling customized building blocks into materials with tailored properties opens doors to explore novel phenomena. Recent advances in incorporating chiral organic cations have given rise to chiral metal-halide semiconductors. These materials exhibit intriguing properties such as chiroptical activity and chirality-induced spin selectivity, enabling the generation and detection of circularly polarized light and spin-polarized electrons for applications in spintronics and quantum information.

However, understanding the structural origin of chiroptical activity presents a challenge due to macroscopic factors and experimental constraints.

In our study [1], we present an achiral perovskite derivative $[Cu_2(pyz)_3(MeCN)_2][Bi_3I_{11}]$ (pyz = pyrazine; MeCN = acetonitrile), which displays remarkable circular dichroism (CD) arising from the material's non-centrosymmetric structure. It features a unique crystal structure as a polythreaded iodido bismuthate, where $[Bi_3I_{11}]^{2-}$ chains are threaded through a cationic two-dimensional coordination polymer. The material exhibits a low, direct optical band gap of 1.70 eV. Notably, single crystals exhibit both linear and circular optical activity with a substantial anisotropy factor of up to 0.16. Intriguingly, despite the absence of chiral building blocks, CuBiI exhibits a substantial degree of circularly polarized photoluminescence, reaching 4.9%. This value is comparable to the results achieved by incorporating chiral organic molecules into perovskites, typically ranging from 3% to 10% at zero magnetic field.

Our findings shed light on the macroscopic origin of CD and provide valuable insights for the design of materials with high chiroptical activity.

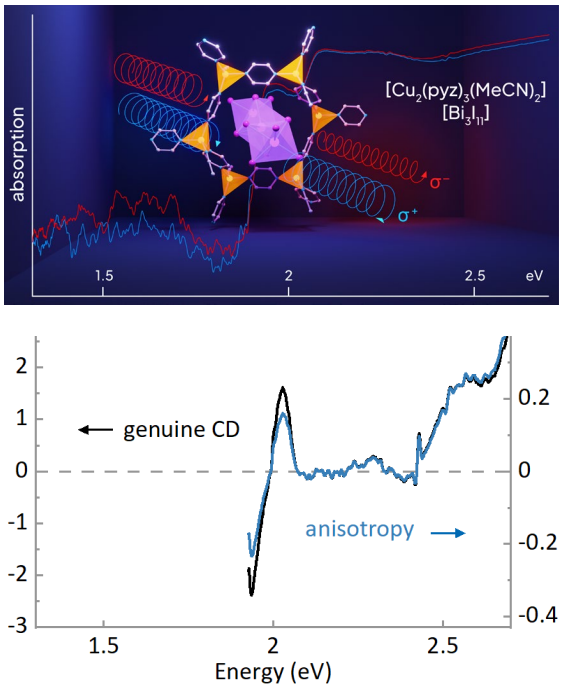

Fig.1. Top: graphic visualization of the compound's structure and circularly polarized absorption spectra. Bottom: genuine circular dichroism (CD) spectrum and anisotropy factor

References

[1] J. Möbs et al., J. Am. Chem. Soc. **145**, 23478-23487 (2023).