Scilight

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What gives the transparent semiconductor copper iodide its color

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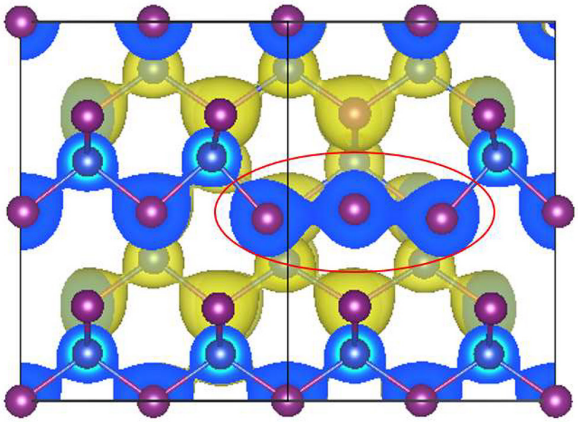
Researchers combined optical experiments with density functional theory to define the off-center model that explain the differences in copper iodide crystal photoluminescence and absorption.



Transparent semiconductors and transistors have found widespread use among various technologies we use today, including, digital displays and photovoltaics. Copper iodide (CuI) has shown promise for light emitting devices as well as perovskite and solid-state dye sensitized solar cells. Most reports, however, have found CuI crystals to be colored, the source of which was unclear.

Koyasu et al. report findings from optical experiments on CuI demonstrating the cause crystals coloration. By evaluating the optical absorption and photoluminescence properties of copper-rich, iodine-rich and pure CuI, the group investigated the relationship between optical properties and native crystal defects. The researchers used an off-center model derived from density functional theory to explain the origin of discrepancies in optical absorption and photoluminescence.

Absorption signals at 2.9 eV and 2.7 eV and a photoluminescent peak at 2.9 eV were observable among iodine-rich samples. A photoluminescent peak at 1.8 eV was dominant in the copper-rich sample.

The authors suggest that the lower-energy absorbance derives from the transition from the crystal's valence band to antisites of iodine substituted for copper, a finding they state can be explained by the off-center model of substituted iodine ions.

CuI has been seen as an attractive material for next-generation solar cells because its synthesis allows for it to be applied to flexible solar cells and that its large lattice parameter provides room for the heteroepitaxial growth required for metal-halide perovskite cells. The authors hope their findings will point to more widespread use of CuI as a substrate for transparent semiconductors.

Source: "Optical properties of single crystalline copper iodide with native defects: Experimental and density functional theoretical investigation," by Satoshi Koyasu, Naoto Umezawa, Akira Yamaguchi, and Masahiro Miyauchi, *Journal of Applied Physics* (2019). The article can be accessed at https://doi.org/10.1063/1.5082865.