Title

Synthesis, structure, and luminescence properties of a 0D organic-inorganic cadmium iodide: Combined experimental and theoretical approach

Abstract

Hybrid organic-inorganic metal halide materials with zero-dimensional (0D) structures have emerged as a captivating field of research due to their distinctive electronic properties and remarkable broadband emission characteristics. In this study, we successfully synthesized a novel hybrid cadmium iodide compound, (BZA)2CdI4.H2O (BZA+: benzylammonium), in the form of single crystals employing the solvent-evaporation method. The room temperature single-crystal X-ray diffraction analysis revealed that (BZA)2CdI4.H2O possesses a typical 0D crystal structure, where (CdI4)2− anions are spatially isolated and surrounded by (BZA)+ cations and H2O molecules. The crystal packing is intricately governed by various non-covalent intermolecular interactions, including π–π stacking interactions, N–H…I, N–H…O, and O–H…I hydrogen bonds, quantified through Hirshfeld surface analysis. Thermal analysis further demonstrated that the removal of water molecules in the crystal lattice yields a dehydrated phase of (BZA)2(CdI4). Upon 330 nm irradiation, the title compound displayed a broad bluish-white light emission, featuring a primary band at 430 nm and a secondary band at 500 nm. Based on photoluminescence spectra measurements and density functional theory (DFT) calculations, the dual-band emission is assigned to the emission of (BZA)+ organic cations and to excitons confined in the [CdI4]2– isolated inorganic tetrahedron, respectively. Interestingly, the presence of isolated molecular units in the 0-D structure results in strongly localized charges and bluish-white light emission with Commission International de l'Eclairage (CIE) colour coordinates (0.23, 0.28). These results confirm the promise of 0D metal-halide hybrids with dual-band emission as

luminescent materials for solid-state lighting.

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Year

2024

Source title

Journal of Molecular Structure

Volume

1314.0

Art. No.

138683

DOI

10.1016/j.molstruc.2024.138683

Link

https://www.scopus.com/inward/record.uri?eid=2-s2.0-85195019662&doi=10.1016%2fj.molstruc.2024.138683&partnerID=40&md5=66ac53fc77cf941a745184f7d79c81cb

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Author Keywords

0D organic metal halides; DFT calculations; Hirshfeld surface analysis; Optical absorption; Photoluminescence properties; Thermal analysis; X-ray diffraction

Index Keywords

Cadmium compounds; Crystal structure; Density functional theory; Electronic properties; Hydrogen bonds; Light absorption; Metal analysis; Metal halides; Molecules; Organic-inorganic materials; Photoluminescence; Positive ions; Single crystals; Thermoanalysis; 0d organic metal halide; Band emission; Density-functional theory calculations; Dual Band; Hirshfeld surface analyse; Hirshfeld surfaces; Organic metals; Photoluminescence properties; White light emission; X- ray diffractions; Surface analysis

Funding Details

Deanship of Scientific Research, Imam Mohammed Ibn Saud Islamic University; Al-Imam Muhammad Ibn Saud Islamic University, IMSIU, (IMSIU-RP23011); Al-Imam Muhammad Ibn Saud Islamic University, IMSIU; Spanish Government, (PGC2018-098630-B-I00)

Funding Texts

Funding text 1: This work was supported and funded by the Deanship of Scientific Research at Imam Mohammad Ibn Saud Islamic University (IMSIU) (grant number IMSIU-RP23011). ECS acknowledges the financial support from the Spanish Government, (Grant PGC2018\u2013098630-B-I00).; Funding text 2: This work was supported and funded by the Deanship of Scientific Research at Imam Mohammad Ibn Saud Islamic University (IMSIU) (grant number IMSIU-RP23011). ECS acknowledges the financial support from the Spanish Government , (Grant PGC2018-098630-B-I00).

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Publisher

Elsevier B.V.

ISSN

00222860

CODEN

JMOSB

Language of Original Document

English

Abbreviated Source Title

J. Mol. Struct.

Document Type

Article

Publication Stage

Final

Source

Scopus

EID

2-s2.0-85195019662