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| Title: | Electron–Phonon Coupling Mediated Self-Trapped-Exciton Emission and Internal Quantum Confinement in Highly Luminescent Zero-Dimensional (Guanidinium)6Mn3X12 (X = Cl and Br) |
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| Keywords: | Electron–Phonon Coupling<br>Self-Trapped-Exciton Emission<br>Internal Quantum Confinement<br>Highly Luminescent Zero-Dimensional |
| Issue Date: | 2022 |
| Publisher: | ACS Publications |
| Citation: | Inorganic Chemistry, 61(43), 17026- 17036. |
| Abstract: | We report a large Stokes shift and broad emission band in a Mn-based organic–inorganic hybrid halide, (Guanidinium)6Mn3Br12 [GuMBr], consisting of trimeric units of distorted MnBr6 octahedra representing a zero-dimensional compound with a liquid like crystalline lattice. Analysis of the photoluminescence (PL) line width and Raman spectra reveals the effects of electron–phonon coupling, suggestive of the formation of Frenkel-like bound excitons. These bound excitons, regarded as the self-trapped excitons (STEs), account for the large Stokes shift and broad emission band. The excited-state dynamics was studied using femtosecond transient absorption spectroscopy, which confirms the STE emission. Further, this compound is highly emissive with a PL quantum yield of ~50%. With chloride ion incorporation, we observe enhancement of the emissive properties and attribute it to the effects of intrinsic quantum confinement. Localized electronic states in flat bands lining the gap and their strong coupling with phonons are confirmed with first-principles calculations. |
| Description: | Only IISER Mohali authors are available in the record. |
| URI: | https://doi.org/10.1021/acs.inorgchem.2c01581 (https://doi.org/10.1021/acs.inorgchem.2c01581)<br>http://hdl.handle.net/123456789/4972 (http://hdl.handle.net/123456789/4972) |
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