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Optical Band Gap Tuning in Mixed B-site and X-site Aziridinium Perovskites

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Three-dimensional hybrid perovskites containing the aziridinium cation (AzrH)BX3 (where AzrH = aziridinium, B is Pb2+ or Sn2+ and X = Cl−, Br−or I−) exhibit semiconductive properties, making them suitable candidates for photovoltaic applications. Small changes in the composition of perovskites are shown to have a defining impact on optoelectronic properties of the reported materials. This study reports the possibility of optical band gap fine-tuning through mixing metals ((AzrH)PbxSn1-xBr3 series) or halogens ((AzrH)PbBrxI3-x series). All the obtained mixed perovskites crystallize in the $Pm\bar{3}m$ space group at room temperature saving their 3D structure. The optical band gap of mixed-metal perovskites varies non-linearly from 1.96 eV to 2.46 eV, while halogen substitution tunes the band gap within the 1.57 −2.23 eV range, as measured by electronic spectroscopy. Additionally, phase transitions and powder X-ray diffraction were used to characterize the structural properties of these compounds. The results expand the scope of hybrid perovskites with tunable band gaps beyond conventional methylammonium and formamidinium-based systems, introducing a new series of metal-halide hybrids with potential applications in photovoltaic and optoelectronic technologies.

Type of presence

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