Multi-length scale structure of 2D/3D Dion–Jacobson hybrid perovskites based on an aromatic diammonium spacer

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Streszczenie

Dion–Jacobson (DJ) iodoplumbates based on 1,4-phenylenedimethanammonium (PDMA) have recently emerged as promising light absorbers for perovskite solar cells. While PDMA is one of the simplest aromatic spacers potentially capable of forming a DJ structure based on (PDMA)$A_{n-1}Pb_nI_{3n+1}$ composition, the crystallographic proof has not been reported so far. Single crystal structure of a DJ phase based on PDMA is presented and high-field solid-state NMR spectroscopy is used to characterize the structure of PDMA-based iodoplumbates prepared as thin films and bulk microcrystalline powders. It is shown that their atomic-level structure does not depend on the method of synthesis and that it is ordered and similar for all iodoplumbate homologues. Moreover, the presence of lower (*n*) homologues in thin films is identified through UV–Vis spectroscopy, photoluminescence spectroscopy, and X-ray diffraction measurements, complemented by cathodoluminescence mapping. A closer look using cathodoluminescence shows that the micron-scale microstructure corresponds to a mixture of different layered homologues that are well distributed throughout the film and the presence of layer edge states which dominate the emission. This work therefore determines the formation of DJ phases based on PDMA as the spacer cation and reveals their properties on a multi-length scale, which is relevant for their application in optoelectronics.

Słowa kluczowe

cathodoluminescence, Dion-Jacobson phases, hybrid perovskites, solid state NMR spectroscopy, structure elucidation