

The effect of precursor concentrations on the structure and optoelectronic properties of the quasi low-dimensional hybrid 2-methylpyridinium lead bromide crystalline phases

D.S. Shtarev^{1,2a,*}, D.A. Chaplygina^{2,b}, O.V. Patrusheva^{2,c}, C. Chen^{3,d}, A.V. Shtareva^{4,e}, C.C. Stoumpos^{5,6,f}, R. Kevorkyants^{6,g}, A.V. Emeline^{6,h}

¹ Shenzhen MSU-BIT University, PRC.

² Institute of High Technologies and Advanced Materials of the Far Eastern Federal University, Russian Federation.

³ Department of Chemistry, Southern University of Science and Technology, PRC.

⁴ Institute of Tectonics and Geophysics, Far Eastern Branch, Russian Academy of Sciences, Russian Federation.

⁵ The Department of Materials Science and Technology, University of Crete, Greece.

⁶ The Laboratory 'Photonics of crystals', Saint-Petersburg State University, Russian Federation.

^a shtarev@mail.ru, ^b chaplygina.dal@dvfu.ru, ^c patrusheva.ov@dvfu.ru, ^d

12331059@mail.sustech.edu.cn, ^e shtareva_anna@mail.ru, ^f cstoumpos@materials.uoc.gr, ^g

r.kevorkyants@spbu.ru, ^h alexei.emeline@spbu.ru

* Corresponding author (ORCID: 0000-0002-1274-0183)

Supplementary material

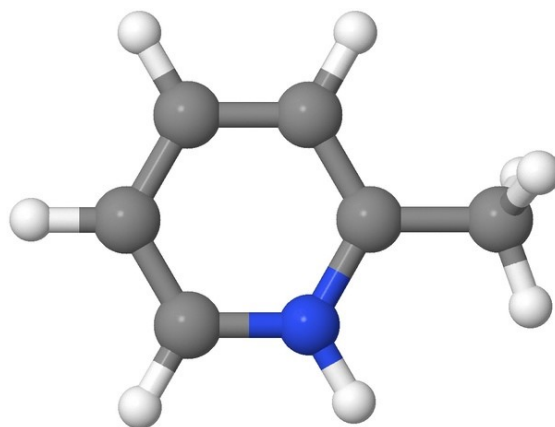


Figure S1. Ball-and-stick model of 2-methylpyridinium cation. The gray, blue, and white balls are carbon, nitrogen, and hydrogen atoms, respectively.

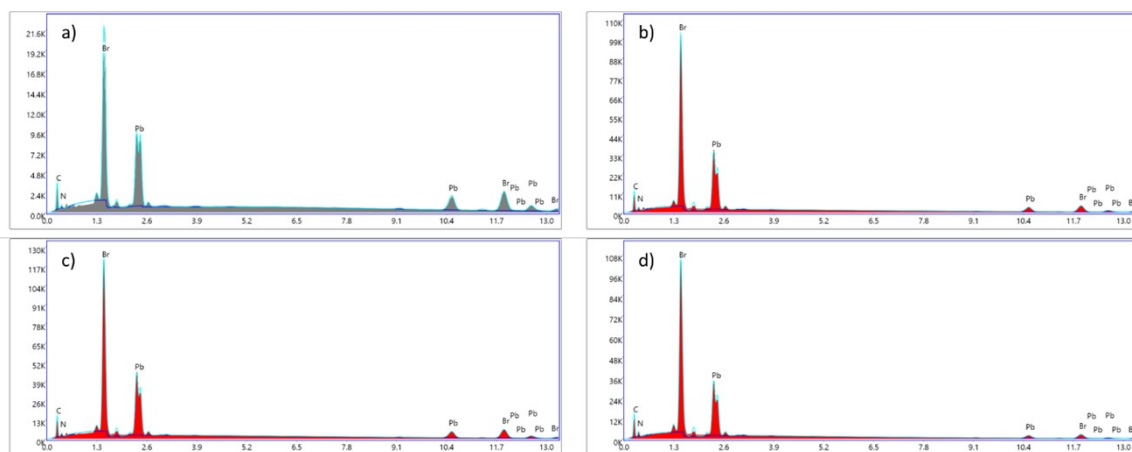


Figure S2. EDX spectra of the precipitate samples prepared with different molar ratios of organic to inorganic moieties: 1:3 (a), 1:2 (b), 1:1 (c), and 2:1 (d).

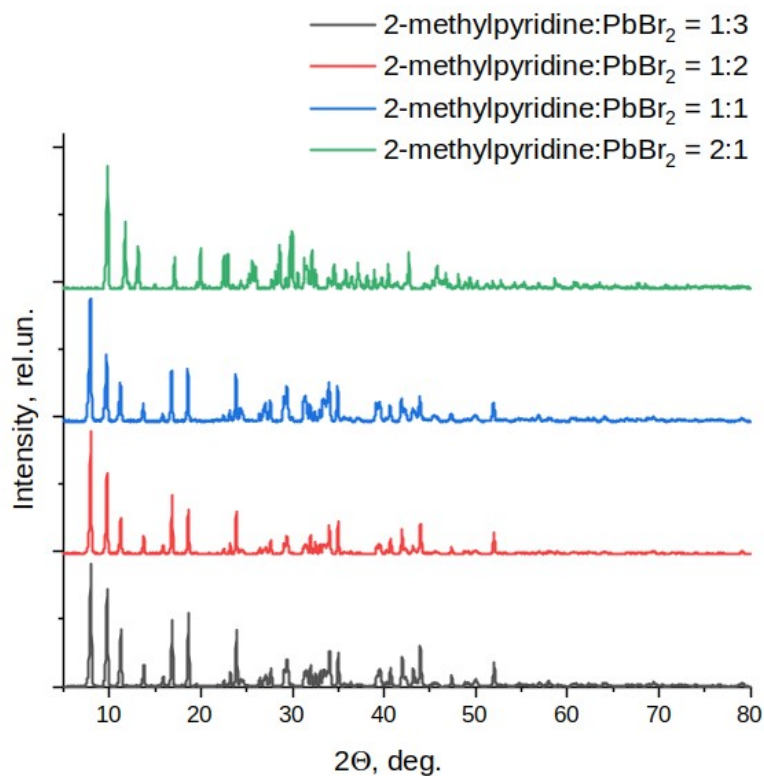


Figure S3. Powder XRD spectra of the 2-methylpyridinium lead bromides prepared with different ratios of reactants.

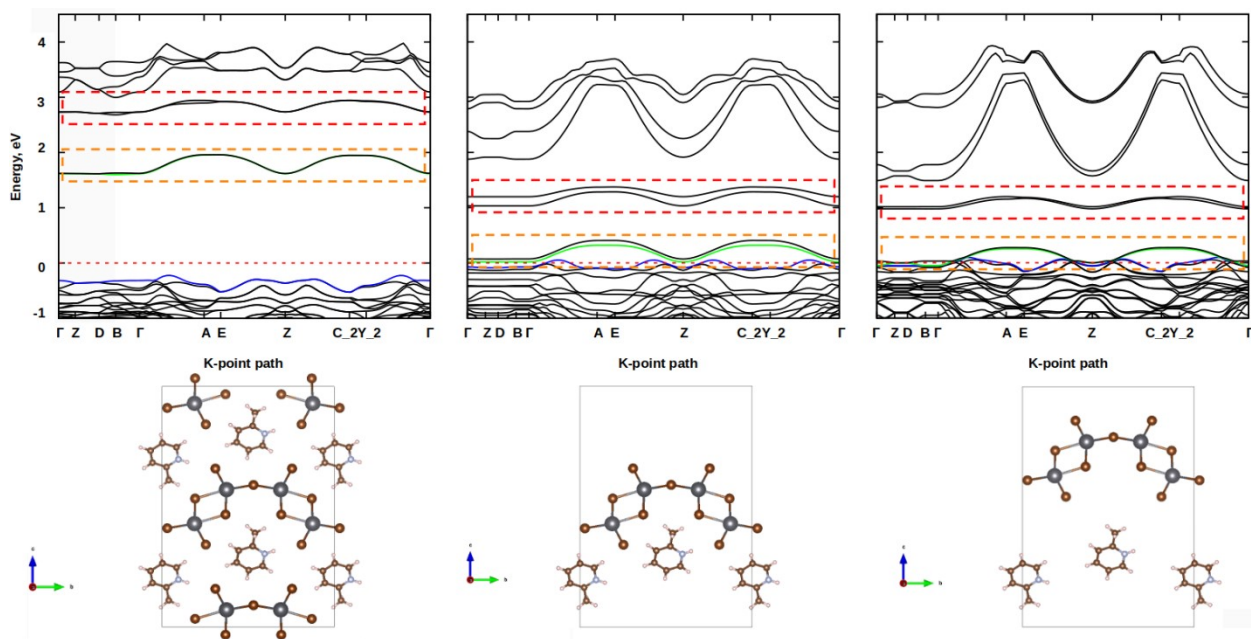


Figure S4. Crystal (top) and electronic (bottom) structures of the Phase-1 2-methylpyridinium lead bromide. Left to right: Original structure, model 1, and model 2. Light brown, small dark brown, large dark brown, blue, and black balls denote H, C, Br, N, and Pb atoms, respectively.

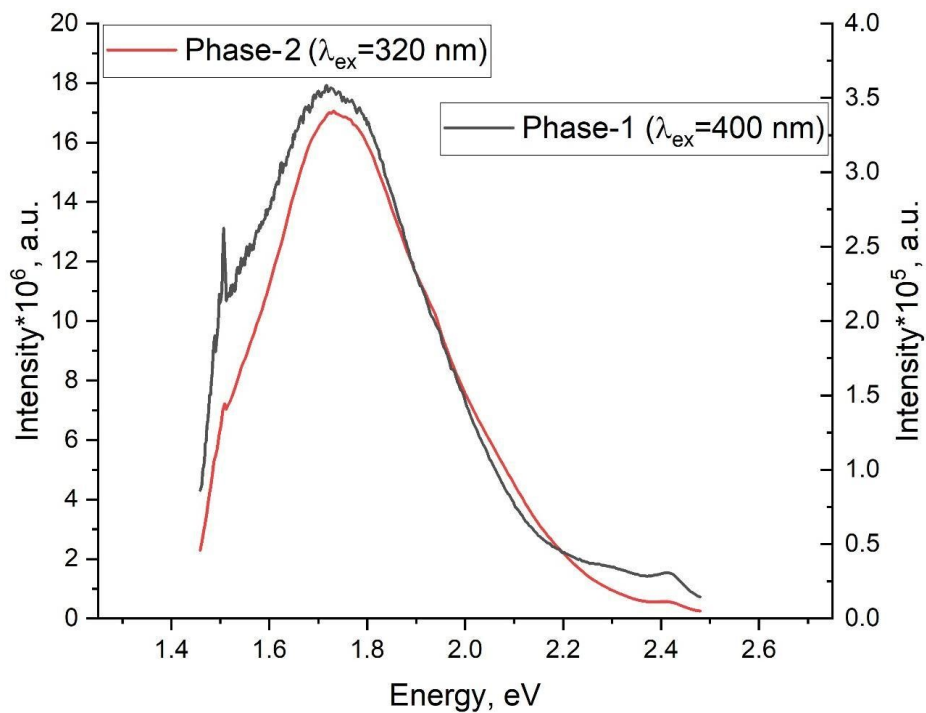


Figure S5. Photoluminescence excitation spectra of the Phase-1 and Phase-2 in the extrinsic absorption region.

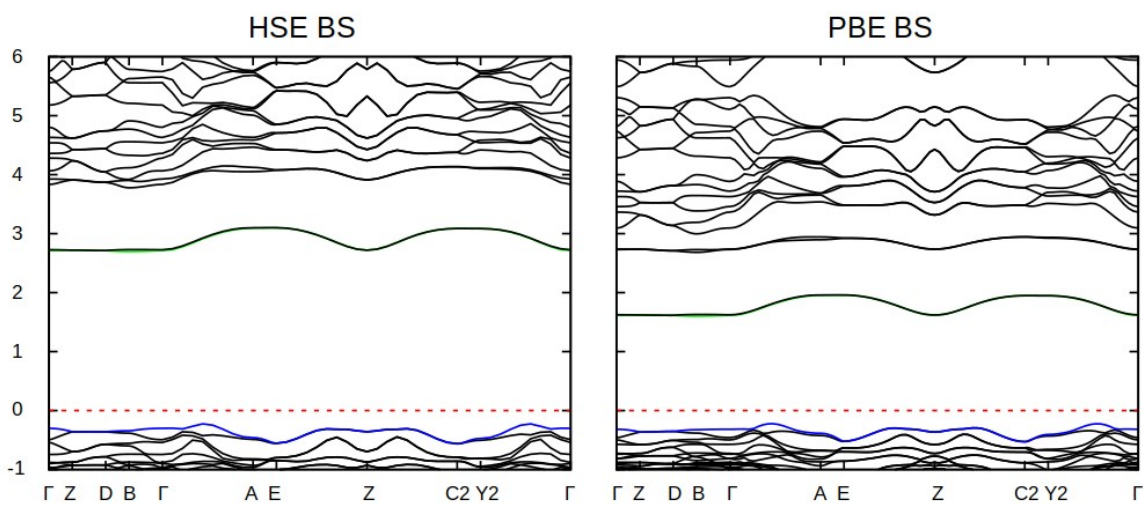


Figure S6. Electronic band structures of the 2-methylpyridinium lead bromide Phase-1: HSE06 (left) and PBE (right).

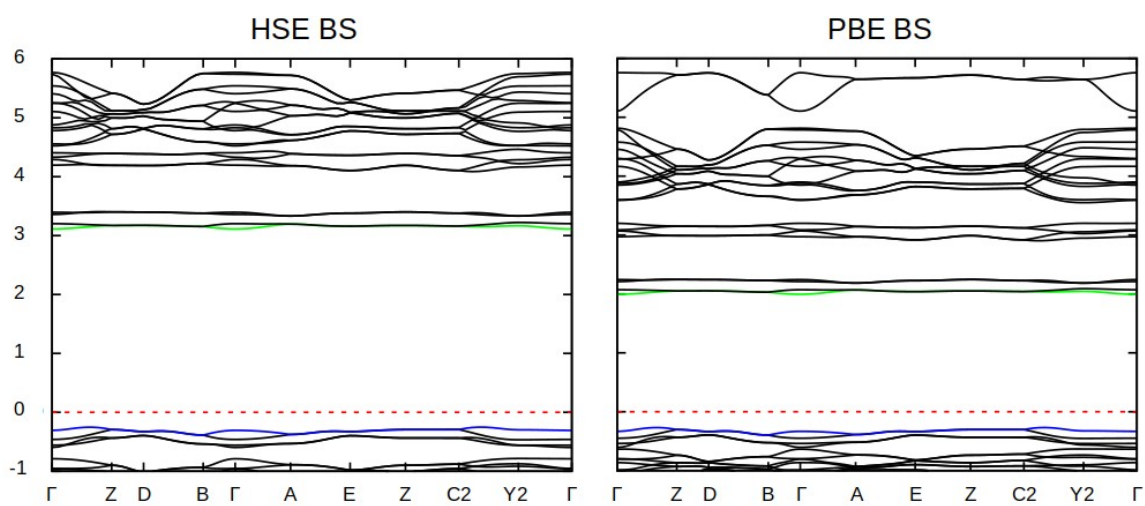


Figure S7. Electronic band structures of the 2-methylpyridinium lead bromide Phase-2: HSE06 (left) and PBE (right).