Electronic supplementary materials *Mendeleev Commun.*, 2025, **35**, 573–576

Towards stable wide-bandgap perovskite absorbers: controlling light-induced halide phase segregation in $CsPbI_2Br$ through partial lead substitution

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Content

Materials and methods

Materials

Glass slides (25x25 mm) used as substrates were purchased from Iso-lab GmbH. Anhydrous dimethyl sulfoxide (DMSO) used as solvent was purchased from Sigma-Aldrich and used as received inside nitrogen glove boxes. The following anhydrous reagents and solvents were purchased from Sigma-Aldrich (USA): CsI, CsBr, PbI_2, CaI_2, SrI_2, BaI_2, PtI_2, EuI_2, SnI_2, MnI_2, FeI2, CoI_2, CuI, AgI, ZnI_2, HgI_2, CdI_2, and SbI_3 (purity 99.999%); YI_3, NdI_3, DyI_2, YbI_2, and LuI_3 (purity 99.9%); GeI_2 (purity 99.8%); MgI_2, BiI_3, and InI_3 (purity 99.998%); NiI_2, LaI3, CeI_3, ErI_3, TbI_3, and GdI_3 (purity 99.99%)

Perovskite films characterization

The UV-Vis absorption spectra were obtained using an AvaSpec-2048-2 UV-Vis fiber spectrometer integrated inside a glove box. The X-ray diffraction (XRD) patterns were collected using an Aeris instrument (Malvern PANalytical B.V.) with the CuKα source.

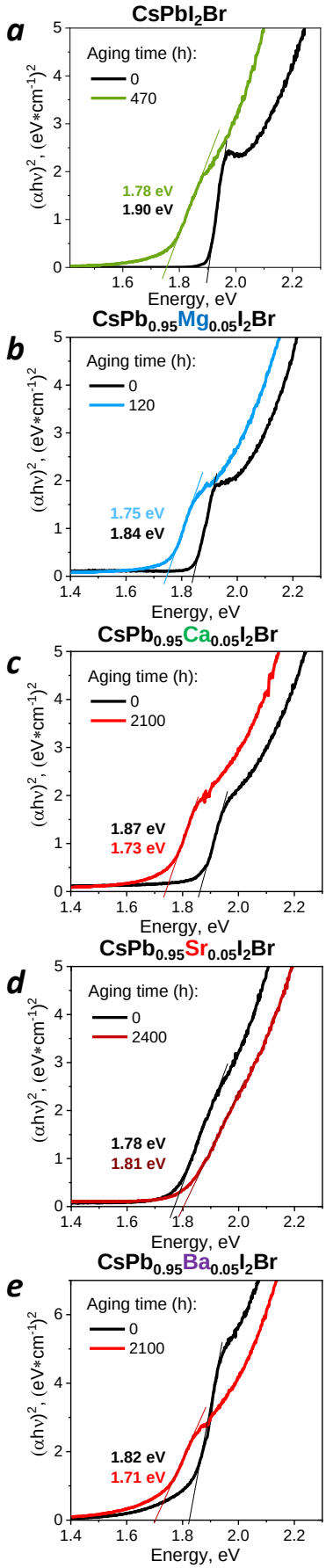

Figure S1. Tauc plots illustrating the change in the band gap of the films $CsPbI_2Br$ (a), $CsPb_{0.95}Mg_{0.05}I_2Br$ (b), $CsPb_{0.95}Ca_{0.05}I_2Br$ (c), $CsPb_{0.95}Sr_{0.05}I_2Br$ (d), and $CsPb_{0.95}Ba_{0.05}I_2Br$ (e).

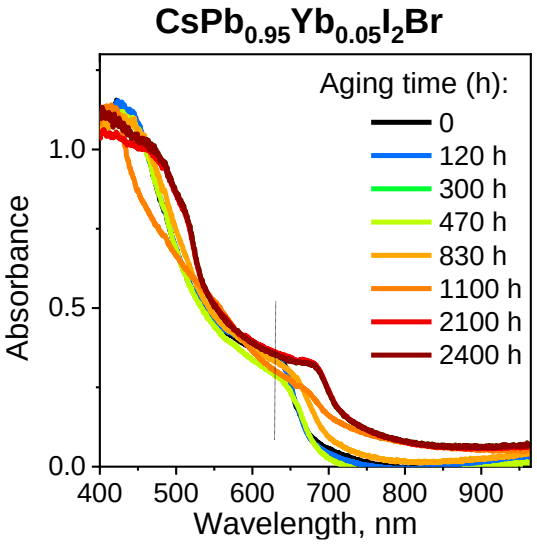

Figure S2. The evolution of the optical UV-Vis absorption spectra of the $CsPb_{0.95}Yb_{0.05}I_2Br$ films during 2400 h of aging.

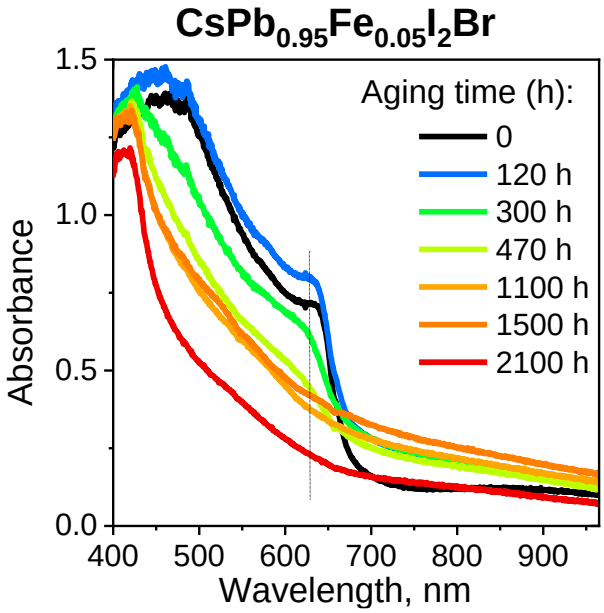

Figure S3. The evolution of the optical UV-Vis absorption spectra of the $CsPb_{0.95}Fe_{0.05}I_2Br$ films during 2100 h of aging.

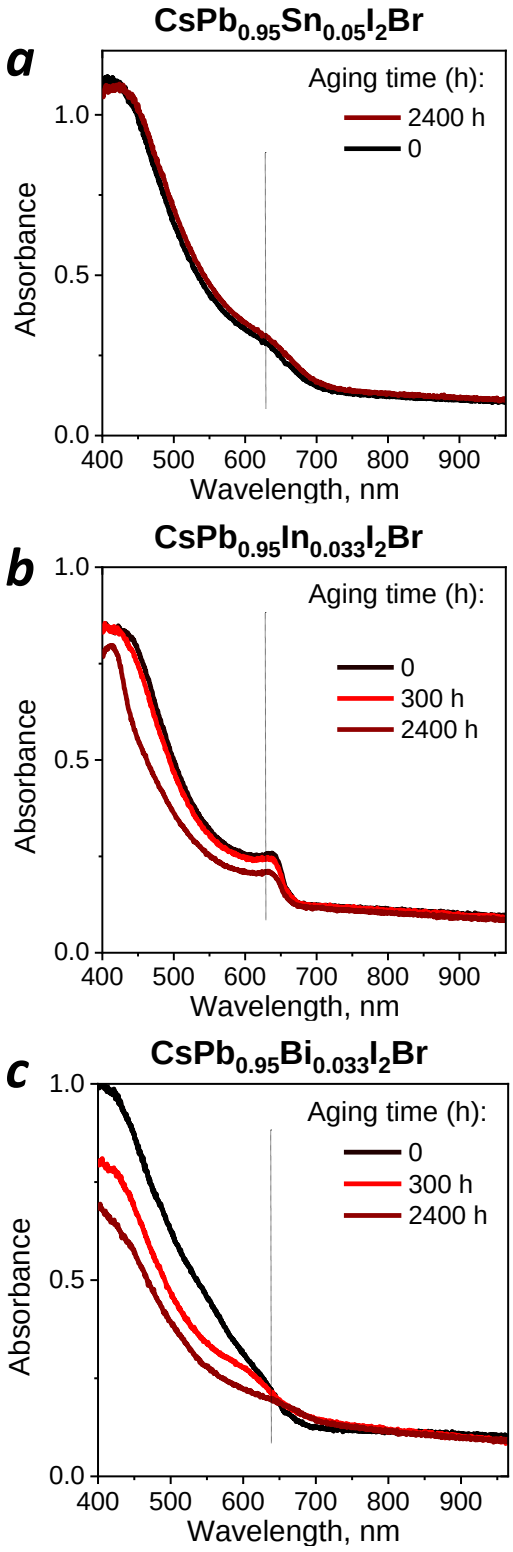

Figure S4. The evolution of the optical UV-Vis absorption spectra of the $CsPb_{0.95}Sn_{0.05}I_2Br$, $CsPb_{0.95}In_{0.033}I_2Br$ and $CsPb_{0.95}Bi_{0.033}I_2Br$ films during 2400 h of aging.

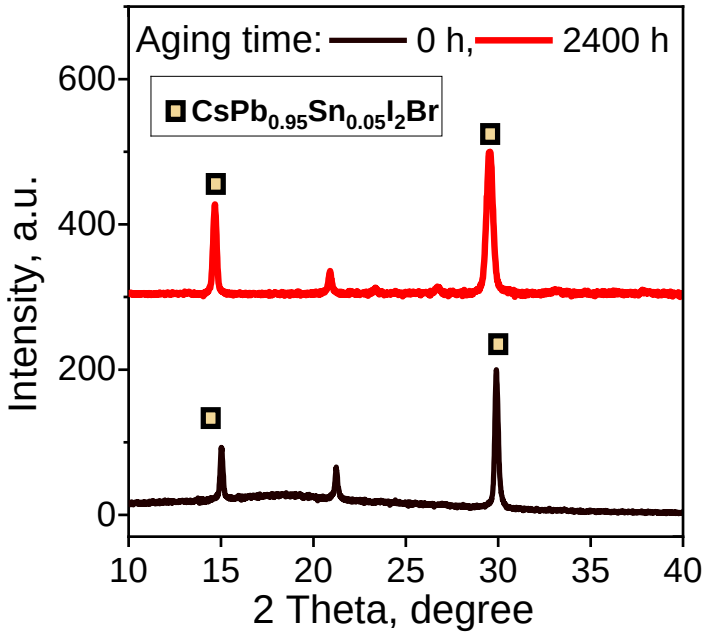

Figure S5. The XRD patterns of the pristine $CsPb_{0.95}Sn_{0.05}I_2Br$ films and after 2400 h of aging.