Probing pressure-induced structural evolution and its impact on the optical behavior of the vacancy-ordered halide double perovskite Rb_2TeBr_6

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Abstract

We investigate the pressure-induced structural and optical evolution of Rb_2TeBr_6, a lead-free halide perovskite derivative, using synchrotron X-ray diffraction, Raman spectroscopy, photoluminescence (PL), and optical absorption measurements. At ambient conditions, Rb_2TeBr_6 crystallizes in a cubic Fm-3m structure that remains stable below 8.0 GPa. Within this pressure range, subtle inter-octahedral rotations emerge, leading to localized deviations from the ideal cubic framework. This pressure-induced octahedral reorientation enhances radiative recombination, resulting in a pronounced increase in PL intensity up to 2.4 GPa, followed by gradual PL quenching due to the activation of nonradiative relaxation pathways at higher pressures. Upon further compression, Rb_2TeBr_6 undergoes a structural transition to an orthorhombic Pnnm phase near 8.0 GPa, followed by a lower symmetry phase above 10.7 GPa and eventual amorphization beyond 25.5 GPa. Optical absorption measurements reveal continuous band-gap narrowing with increasing pressure. These results demonstrate a strong interplay between lattice dynamics, electronic structure, and optical properties in Rb_2TeBr_6, highlighting its potential as a pressure-tunable material for advanced optoelectronic applications.

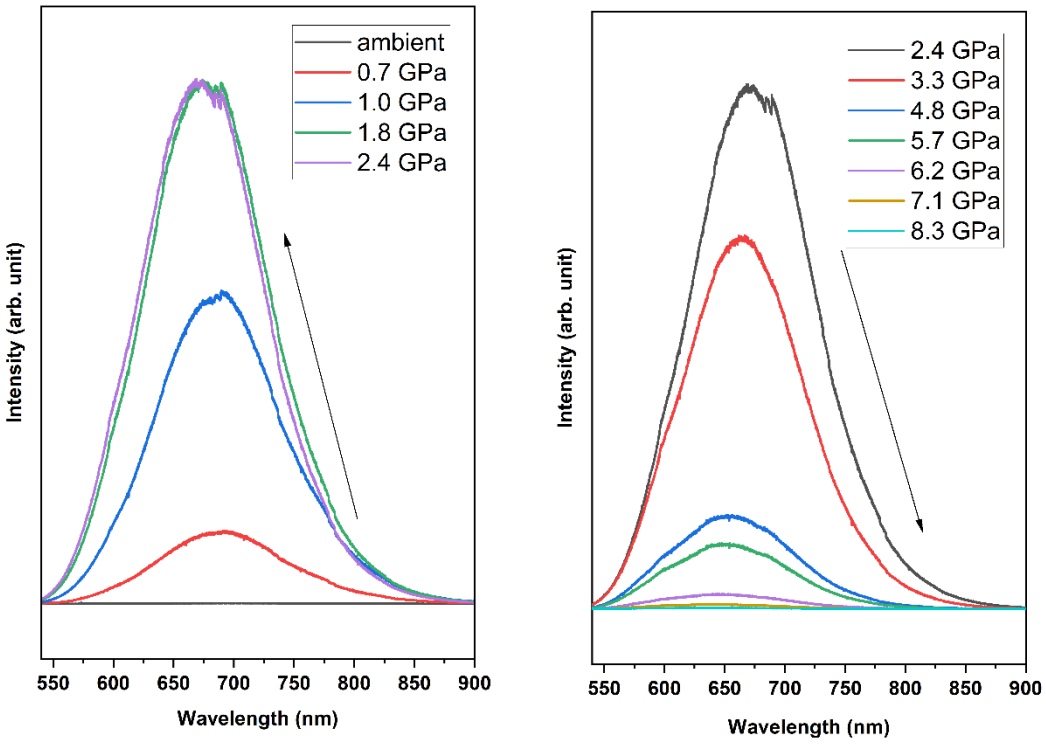

Figure: Photoluminescence (PL) spectra of Rb_2TeBr_6 at selected pressures, showing PL enhancement up to ~2.4 GPa followed by gradual quenching with further compression.