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Supporting Information

Pressure-induced non-radiative losses in halide perovskite light-emitting diodes

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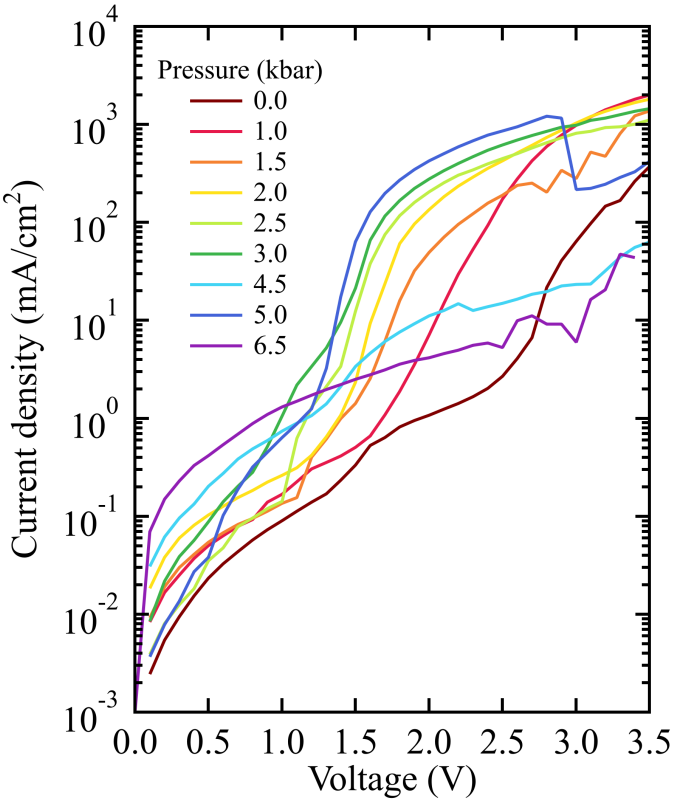

Figure S1: J–V curves measured as a function of applied pressure. At low voltage regime, the current density generally shows a positive correlation with pressure. At high pressure regime, however, a negative correlation is observed.

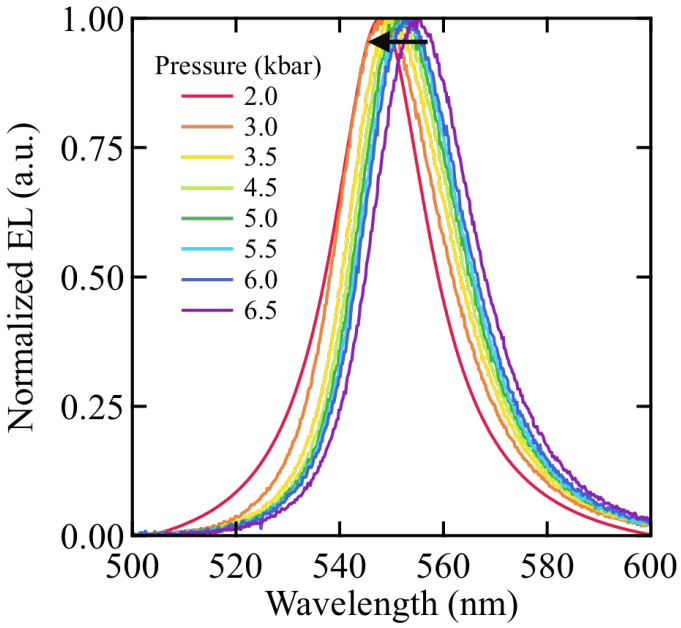

Figure S2: Normalised EL spectra recorded while the pressure on the perovskite $MAPbBr_3$ LED was released gradually. The black arrow shows progression with decreasing pressure. The device clearly displays a gradual return to pre-compression emission peak energies.

Table S1: Result of 3D band structure calculations. P stands for applied pressure to $MAPbBr_3$. k_v^x, k_v^y, and k_v^z indicate exact position of valence band maximum (VBM) in Rashba hole pockets, while k_c^x, k_c^y, and k_c^z indicate exact position of conduction band minimum (CBM) in Rashba electron pockets. Δk_{v} (Δk_{c}) and ΔE_{v} (ΔE_{c}) denote momentum and eigenvalue difference between the R point and exact VBM (CBM), respectively.

P (kbar)	k_v^x	k_v^y	k_v^z	Δk_v (Å^{-1})	ΔE_v (eV)	k_c^x	k_c^y	k_c^z	Δk_c (Å^{-1})	ΔE_c (eV)
0.0	0.512	0.469	0.500	0.03522	0.01597	0.468	0.548	0.500	0.06112	0.08556
0.5	0.512	0.468	0.500	0.03624	0.01639	0.468	0.548	0.500	0.06118	0.08708
1.0	0.512	0.468	0.500	0.03628	0.01692	0.468	0.549	0.500	0.06212	0.08887
1.5	0.512	0.467	0.500	0.03731	0.01734	0.467	0.549	0.500	0.06277	0.09040
2.0	0.513	0.466	0.500	0.03871	0.01811	0.467	0.550	0.500	0.06371	0.09352
3.0	0.513	0.465	0.500	0.03978	0.01926	0.466	0.551	0.500	0.06531	0.09810
4.0	0.514	0.464	0.500	0.04123	0.02032	0.465	0.552	0.500	0.06691	0.10220
5.0	0.515	0.463	0.500	0.04270	0.02149	0.465	0.553	0.500	0.06793	0.10642
6.0	0.515	0.462	0.500	0.04377	0.02271	0.464	0.554	0.500	0.06954	0.11108
7.0	0.516	0.460	0.500	0.04625	0.02387	0.463	0.555	0.500	0.07116	0.11569

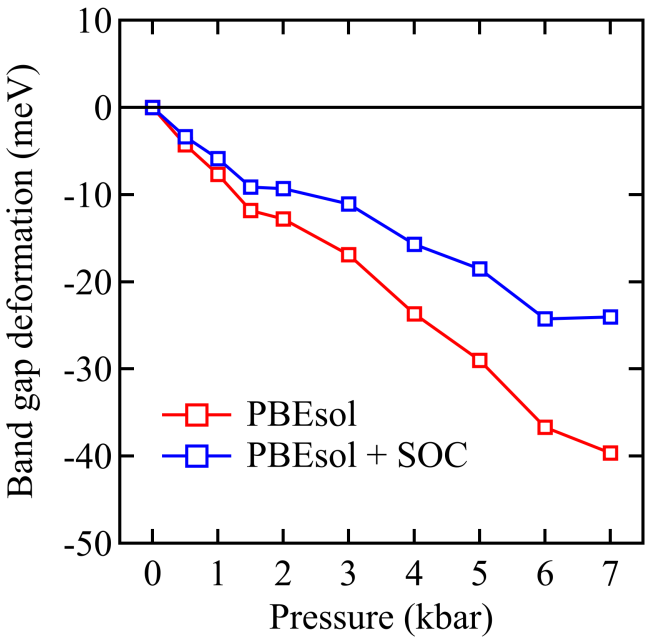

Figure S3: Change in the band gap of $MAPbBr_3$ as a function of pressure. The red squares indicate calculated values from PBEsol functional without spin-orbit coupling (SOC), while the blue squares indicate calculated values from PBEsol with SOC. It is found that the inclusion of SOC mitigates band gap deformation at the given pressure range.

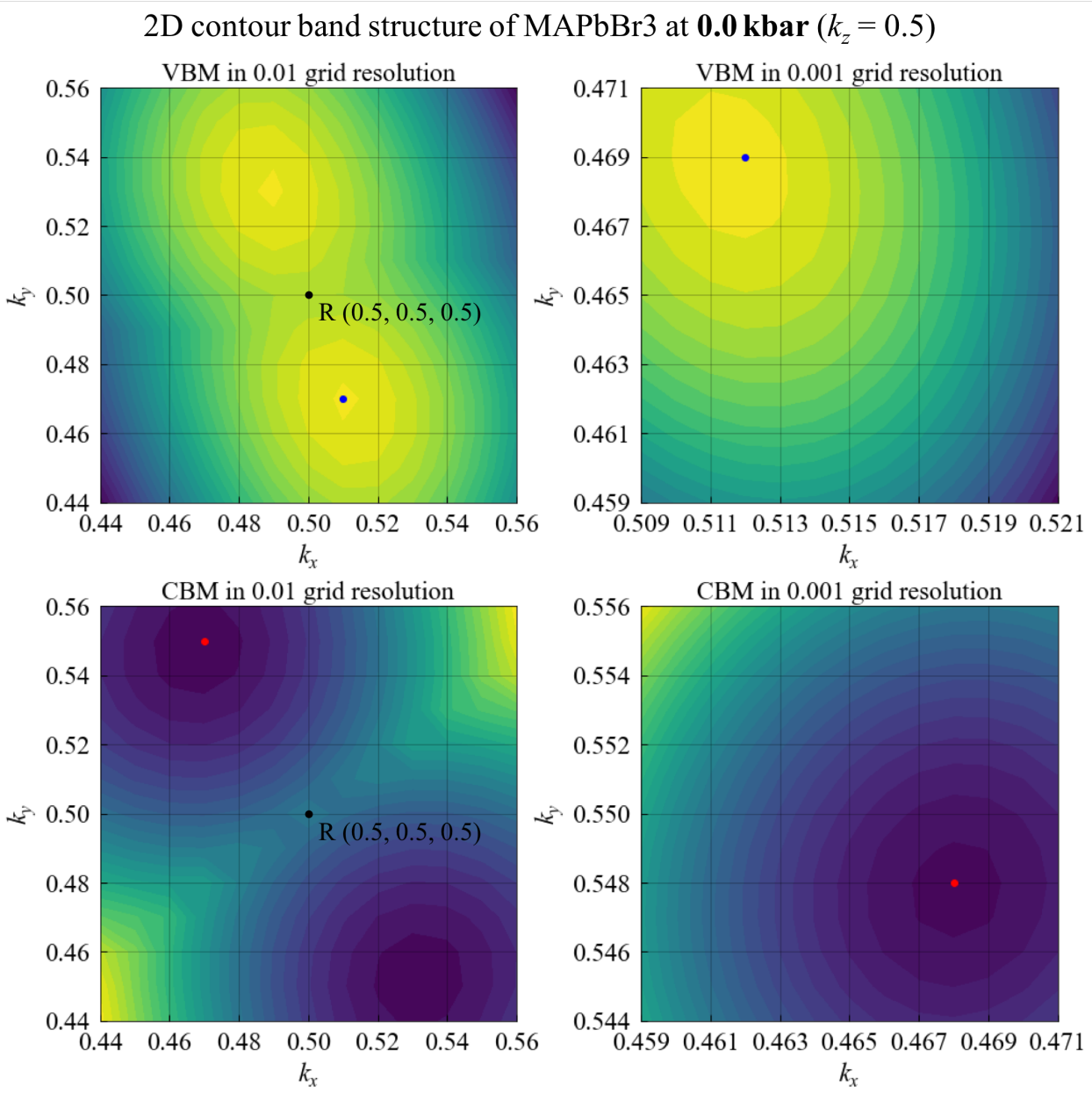

Figure S4: 2D contour plot of upper valence band and lower conduction band of $MAPbBr_3$ near R point in the reciprocal space when compressive hydrostatic pressure of 0.0 kbar is applied. Black dots show the position of R point. Blue dots indicate the position of valence band maximum (VBM) while red dots indicate the position of conduction band minimum (CBM).

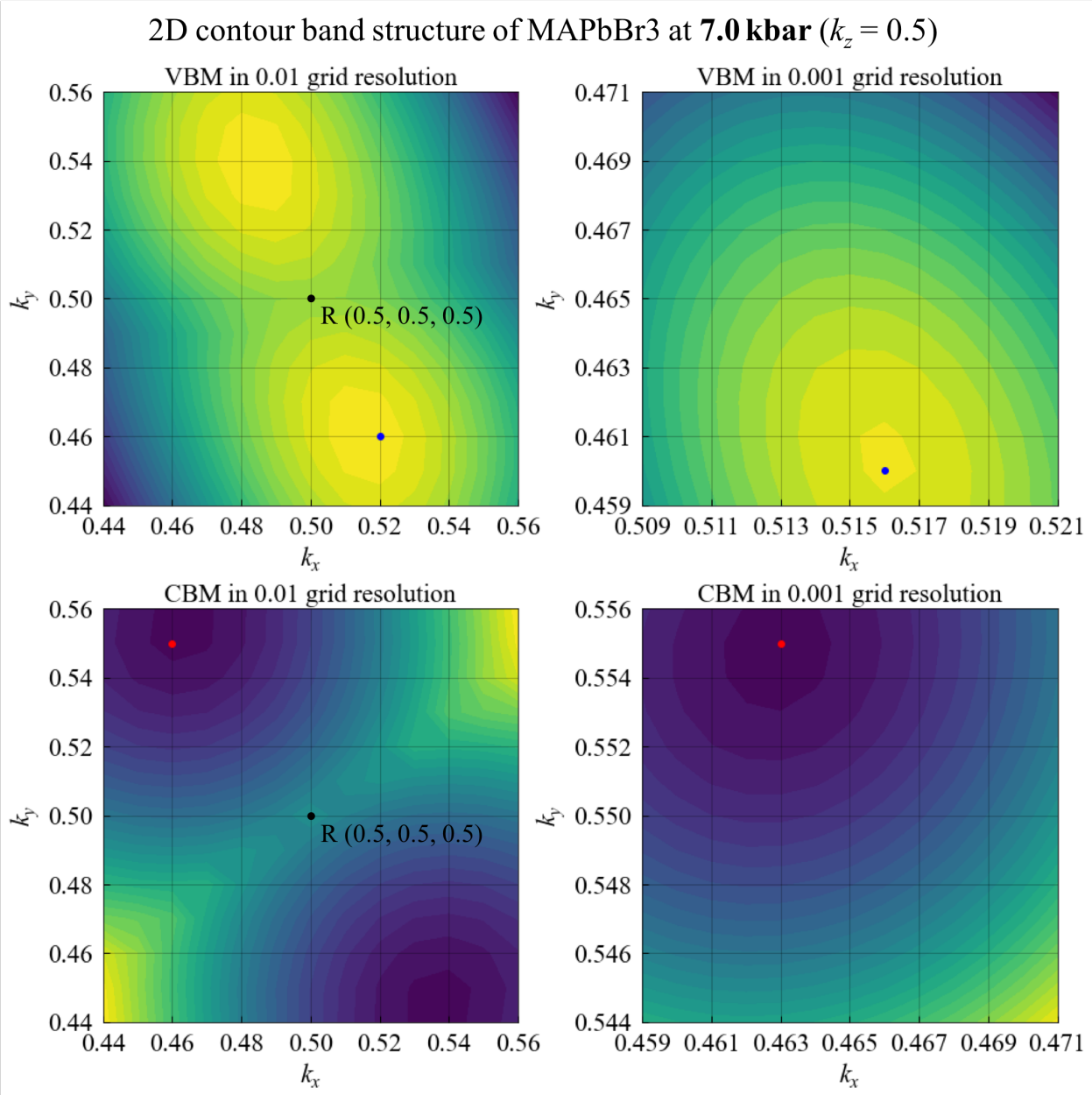

Figure S5: 2D contour plot of upper valence band and lower conduction band of $MAPbBr_3$ near R point in the reciprocal space when compressive hydrostatic pressure of 7.0 kbar is applied. Black dots show the position of R point. Blue dots indicate the position of valence band maximum (VBM) while red dots indicate the position of conduction band minimum (CBM).

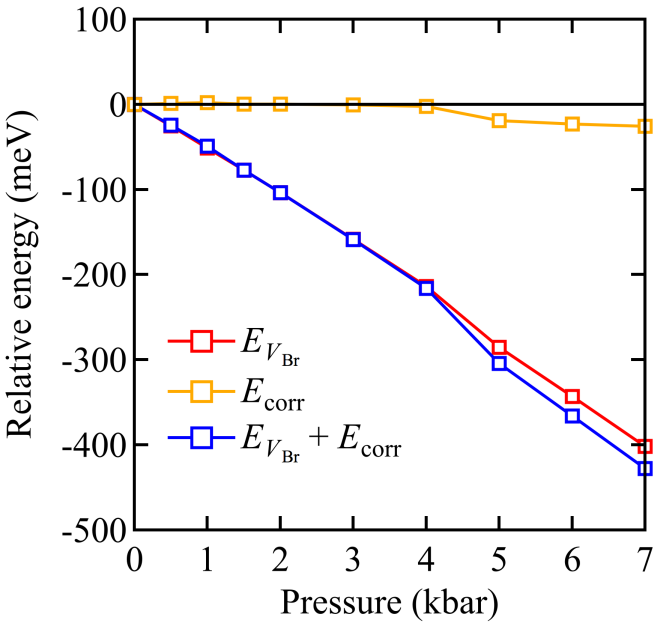

Figure S6: Change in the DFT total energy of defect supercell (red squares) and charged correction term (orange squares) of V_{Br}^{+} as a function of pressure. The blue squares show the sum of the two terms. It is confirmed that the change in charged correction term is negligible at the given pressure range.