Electronic Supplementary Material (ESI) for Materials Advances.

Supporting Information: Phase Transitions in $CsPbBr_3$: Evaluating Perovskite Behavior Over Different Time Scales

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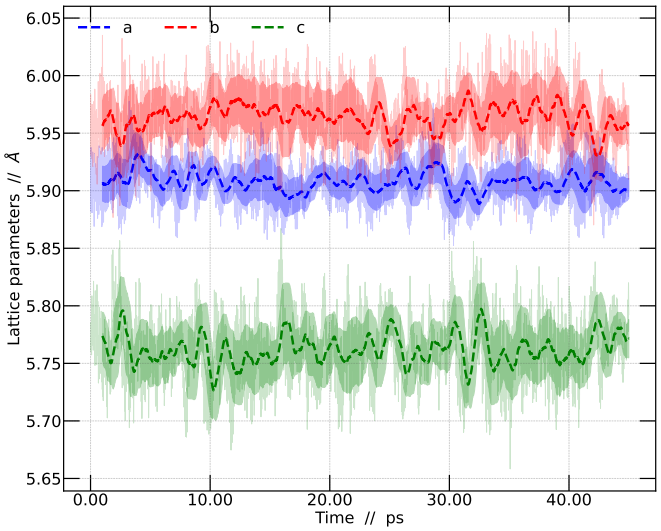

Figure S1: Time evolution of the cell parameters for the perovskite at 150 K. The dashed line indicates the average values calculated in intervals of 1000 fs along with its corresponding standard deviation. The edge a is represented by the blue line, the edge b by the red line, and the edge c by the green line. The shaded region represents the standard deviation around each average.

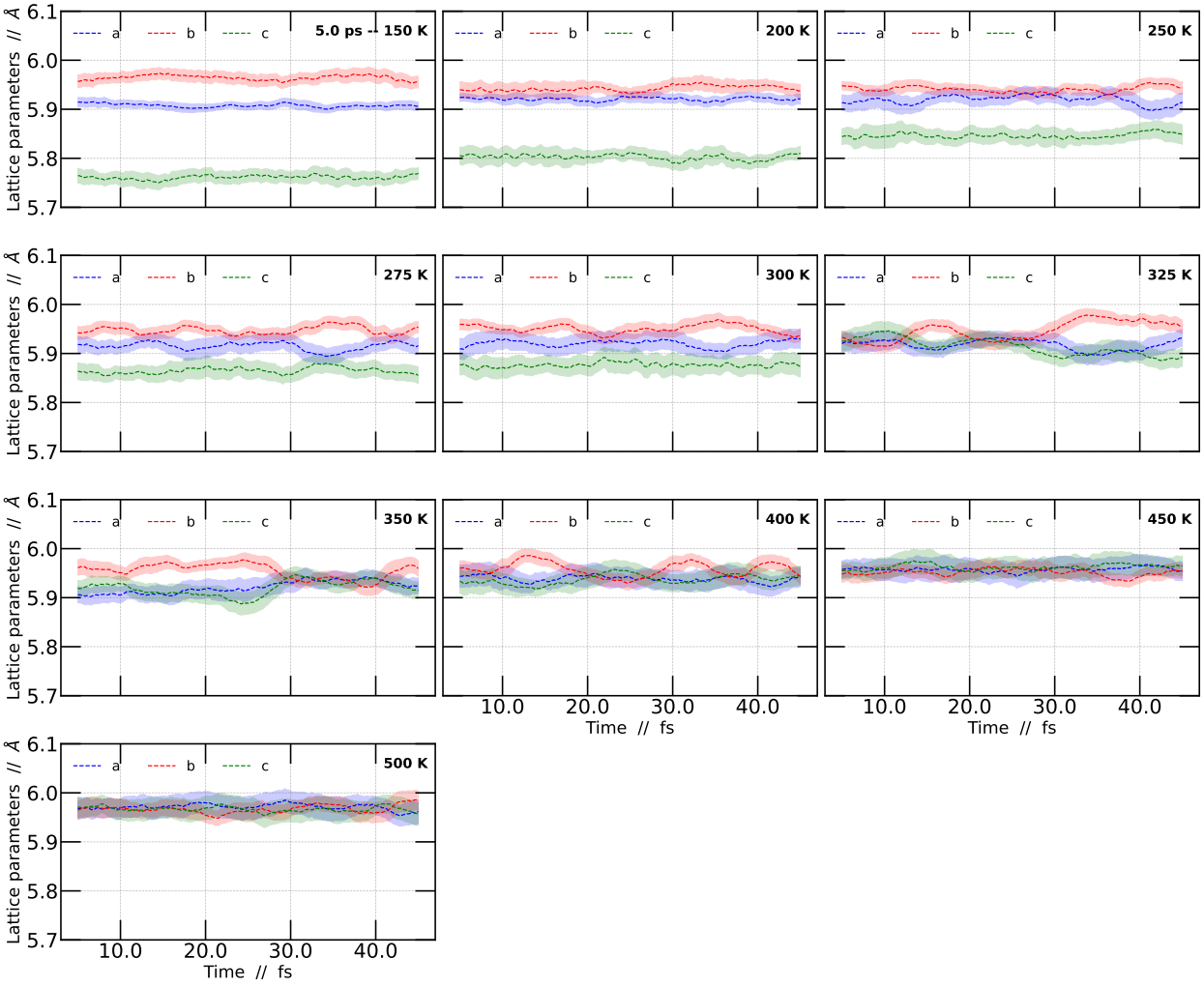

Figure S2: Time evolution of the supercell edges for $CsPbBr_3$ at 150 K, 200 K, 250 K, 275 K, 300 K, 325 K, 350 K, 400 K, 450 K and 500 K. For these graphs, a 5 ps window was used to calculate the average and standard deviation. The edge a is represented by the blue line, the edge b by the orange line, and the edge c by the green line. The shaded region represents the standard deviation around each average.

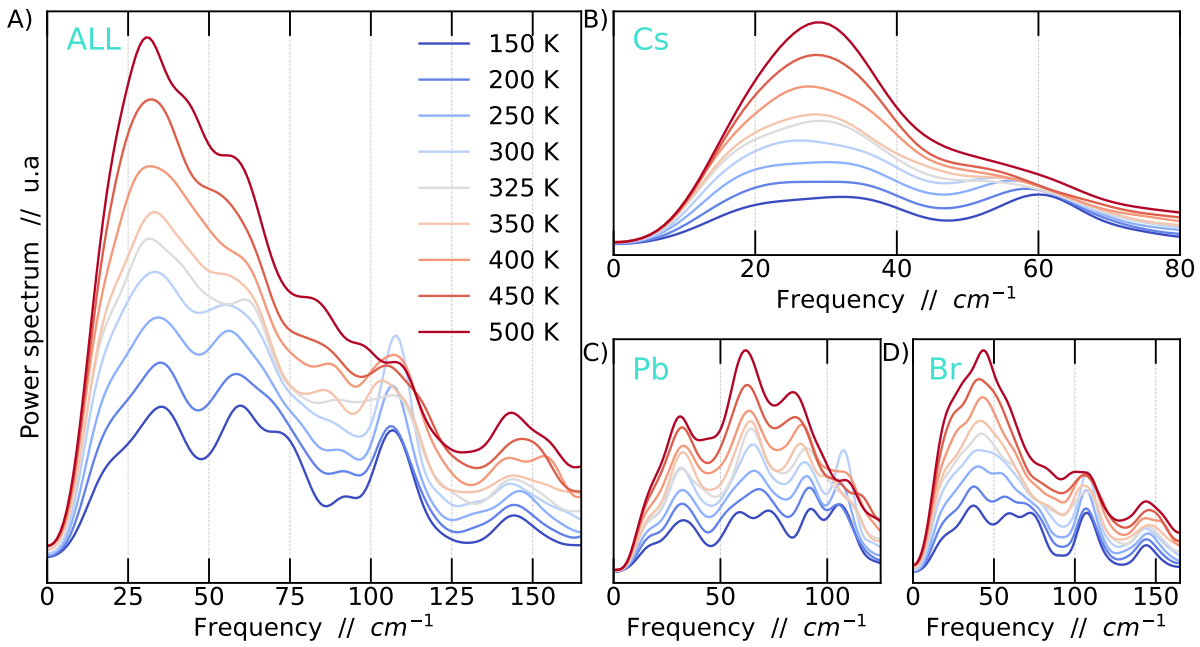

Figure S3: a) Power spectrum as a function of temperature for $CsPbBr_3$ perovskites. The individual contributions of the Cs, Pb and Br atoms are shown in b), c) and d), respectively, sharing the same color scale and y-axis with figure a).