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Physical and Optoelectronic Features of Lead-free $A_2AgRhBr_6$ (A = Cs, Rb, K, Na, Li) with Halide Double Perovskite Composition

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Supplementary Information

Table S1: (Spin-polarized) Cartesian coordinates of SCAN-*rVV*10 relaxed $Cs_2AgRhBr_3$ reduced primitive cell (10 atoms).

	x	y	z
Cs1	0.25000	0.25000	0.25000
Cs2	0.75000	0.75000	0.75000
Ag1	0.50000	0.50000	0.50000
Rh1	0.00000	0.00000	0.00000
Br1	0.23603	0.23603	0.76397
Br2	0.76256	0.76256	0.23744
Br3	0.76256	0.23744	0.76256
Br4	0.23744	0.76256	0.23744
Br5	0.76256	0.23744	0.23744
Br6	0.23744	0.76256	0.76256

Table S2: (Spin-polarized) Cartesian coordinates of SCAN-*rVV*10 relaxed $Cs_2AgRhBr_3$ conventional unit-cell (40 atoms).

	x	y	z
Cs1	0.75000	0.25000	0.75000
Cs2	0.75000	0.75000	0.75000
Cs3	0.25000	0.25000	0.75000
Cs4	0.25000	0.75000	0.75000
Cs5	0.25000	0.25000	0.25000
Cs6	0.75000	0.75000	0.25000
Cs7	0.75000	0.25000	0.25000
Cs8	0.25000	0.75000	0.25000
Ag1	0.50000	0.50000	0.50000
Ag2	0.00000	0.00000	0.50000
Ag3	0.00000	0.50000	0.00000
Ag4	0.50000	0.00000	0.00000
Rh1	0.50000	0.00000	0.50000
Rh2	0.00000	0.50000	0.50000
Rh3	0.50000	0.50000	0.00000
Rh4	0.00000	0.00000	0.00000
Br1	0.50000	0.00000	0.73741
Br2	0.00000	0.50000	0.73741
Br3	0.00000	0.00000	0.76259
Br4	0.50000	0.50000	0.76259
Br5	0.00000	0.26259	0.50000
Br6	0.50000	0.76259	0.50000
Br7	0.00000	0.73741	0.50000
Br8	0.50000	0.23741	0.50000
Br9	0.73741	0.00000	0.50000
Br10	0.23741	0.50000	0.50000
Br11	0.76259	0.50000	0.50000
Br12	0.26259	0.00000	0.50000
Br13	0.50000	0.50000	0.23741
Br14	0.00000	0.00000	0.23741
Br15	0.50000	0.00000	0.26259
Br16	0.00000	0.50000	0.26259
Br17	0.50000	0.73741	0.00000
Br18	0.00000	0.76259	0.00000
Br19	0.50000	0.26259	0.00000
Br20	0.26259	0.50000	0.00000
Br21	0.76259	0.00000	0.00000
Br22	0.00000	0.23741	0.00000
Br23	0.73741	0.50000	0.00000
Br24	0.23741	0.00000	0.00000

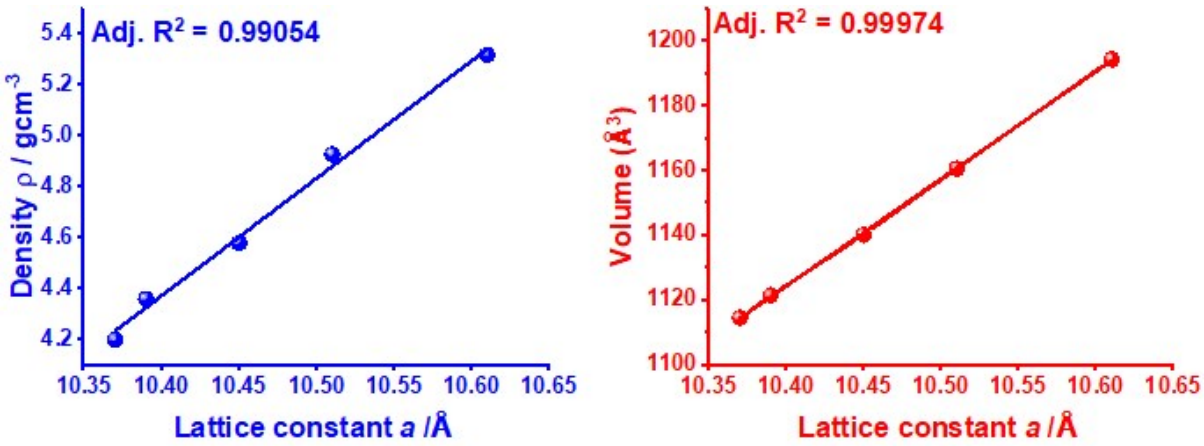

Figure S1: Dependence of a) density, and b) volume of the conventional unit-cell on the lattice constant *a* for $A_2AgRhBr_6$ (*A* = Cs, Rb, K, Na, Li). (See Table 1 for density, volume and lattice constants).

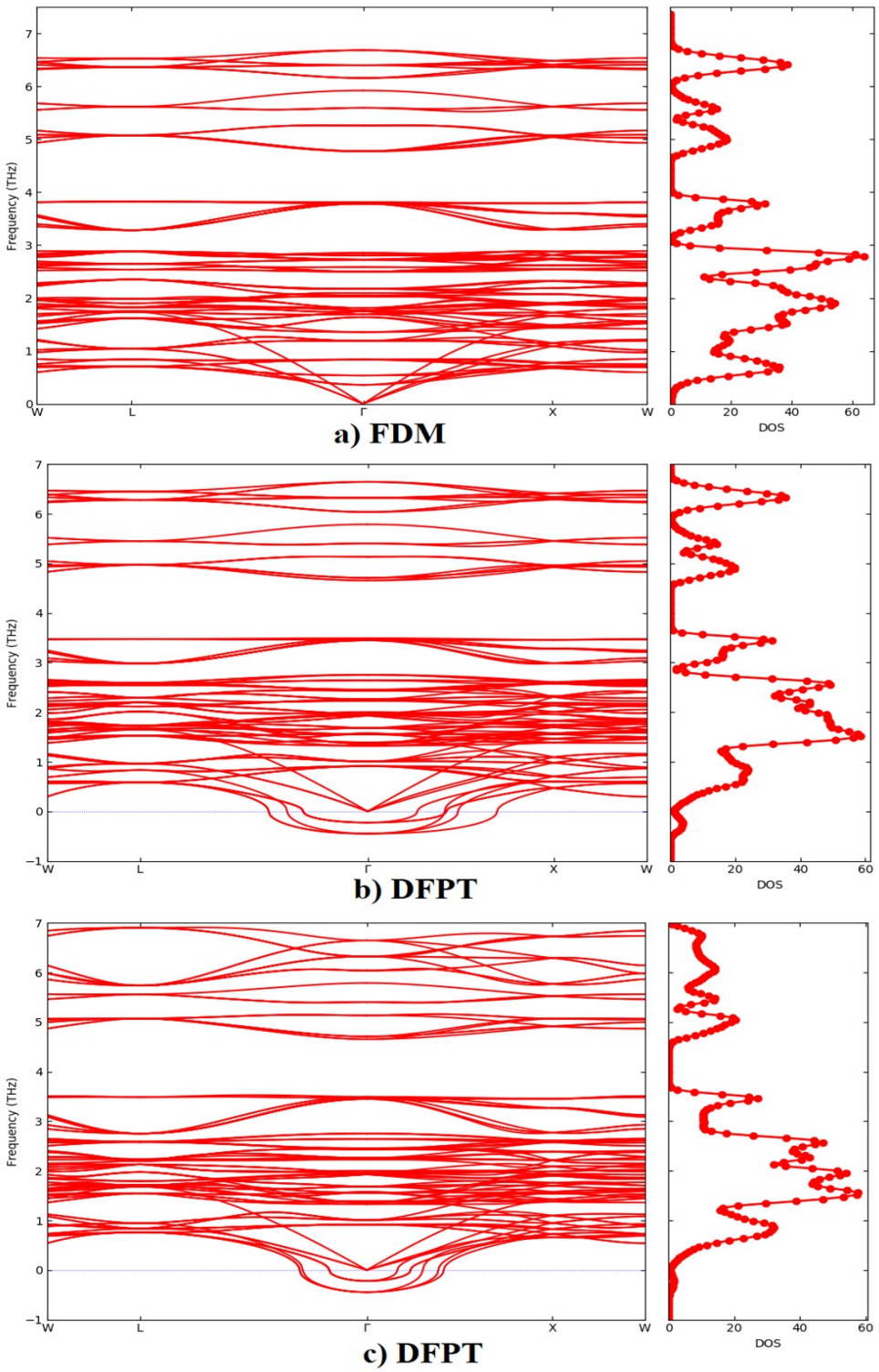

Figure S2. Comparison of the FDM level (harmonic) phonon dispersion, together with total phonon density of states of $Cs_2AgRhBr_6$ with that of DFPT. a) Conventional unit-cell (40 atoms) with FDM; b) Conventional unit-cell (40 atoms) with DFPT; c) 2×2×2 supercell (320 atoms) built of the conventional unit-cell with DFPT.

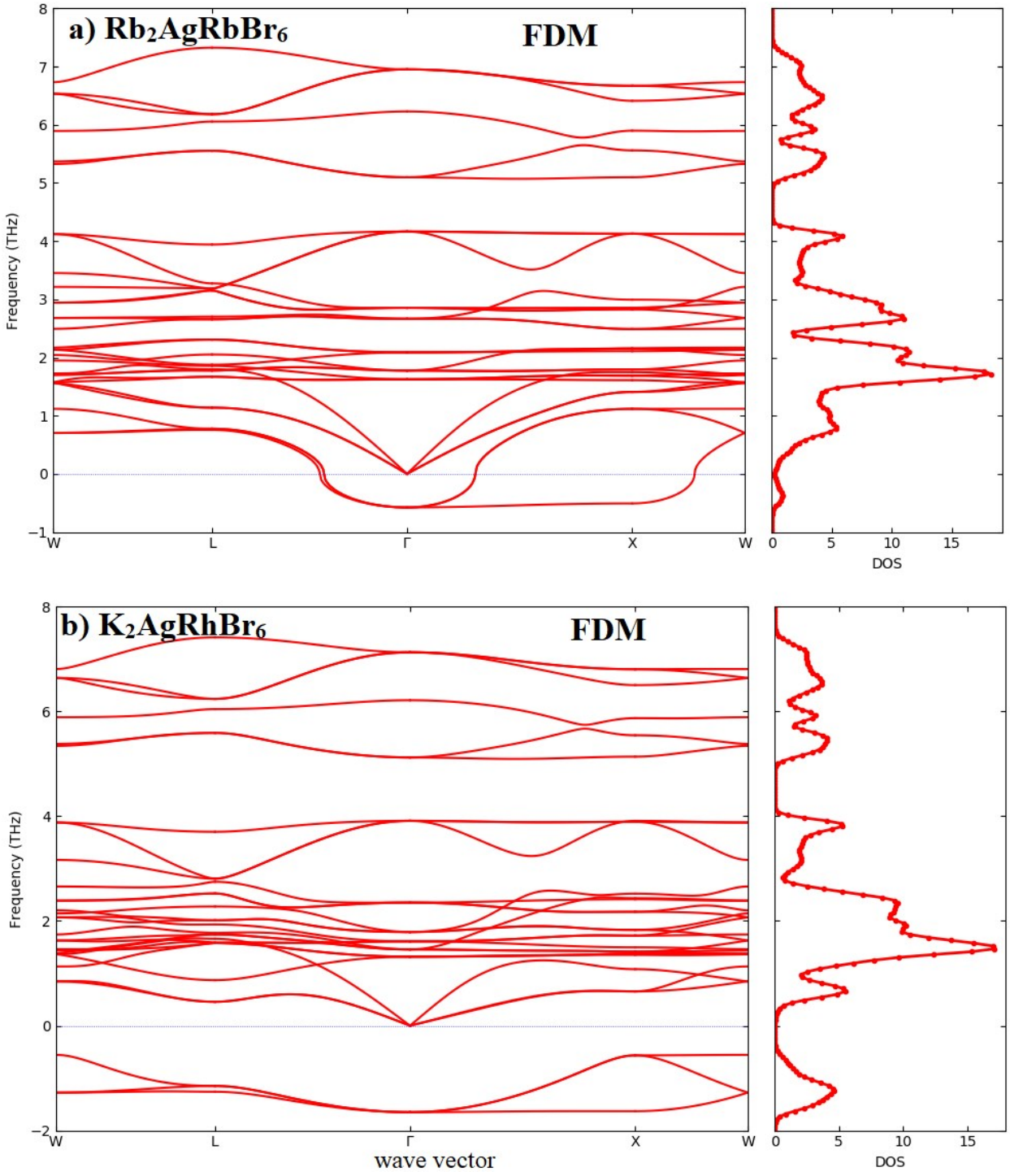

Figure S3. Comparison of the FDM (Finite Different Method) level (harmonic) phonon dispersion, together with total phonon density of states of $Rb_2AgRhBr_6$ with that of $K_2AgRhBr_6$. The 2×2×2 supercells (80 atoms) of both the systems constructed using their corresponding relaxed primitive unit-cells were used.

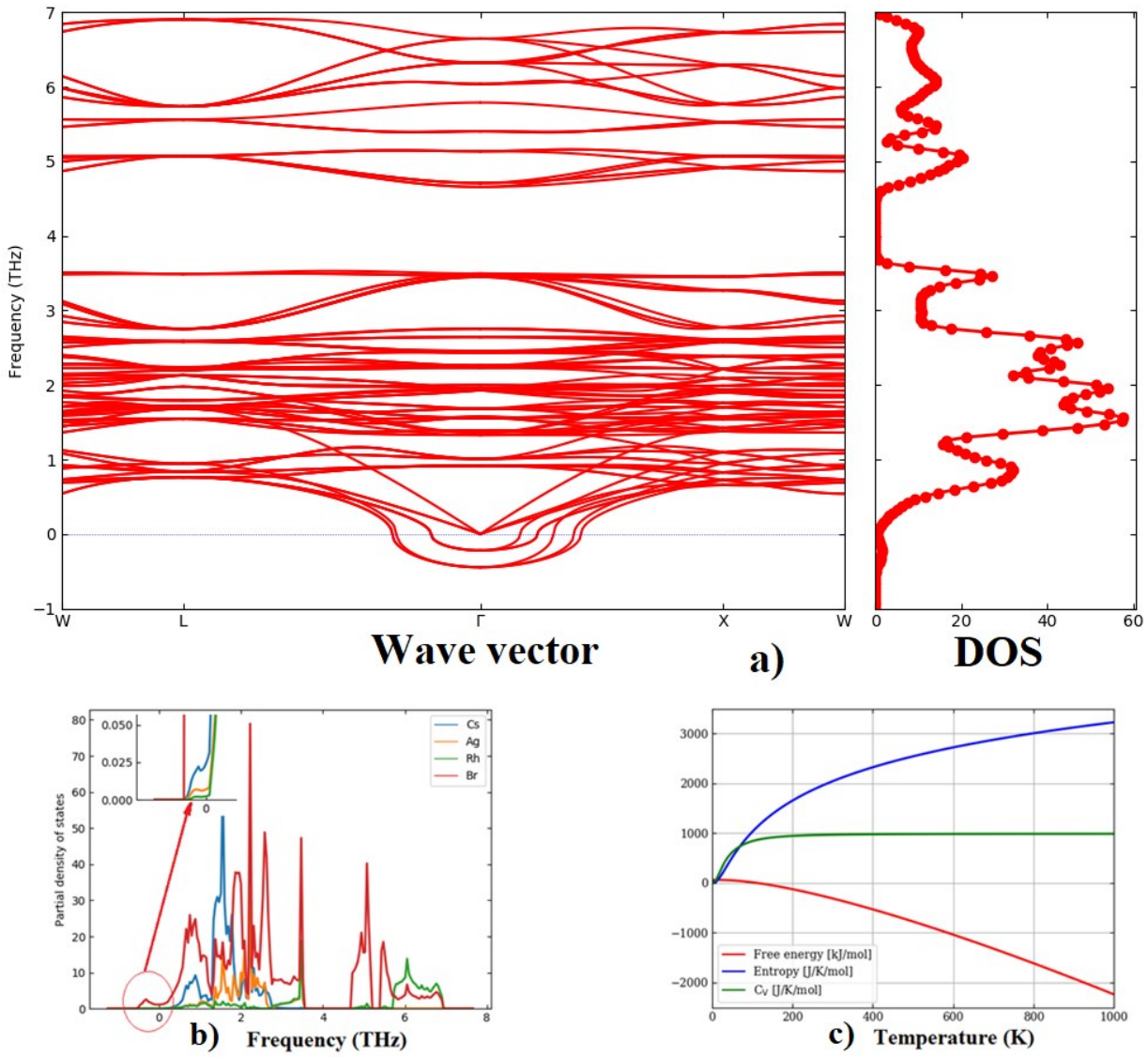

Figure S4. a) (DFPT) Harmonic level phonon dispersion, together with total phonon density of states, b) partial phonon density of states, and c) thermal properties of $Cs_2AgRhBr_6$. The insert in b) marked by an arrow in red refers to the frequency region below 0.0 THz. The 2×2×2 supercell (320 atoms) built of the conventional unit-cell was used. A similar result was obtained with the conventional unit-cell (40 atoms).

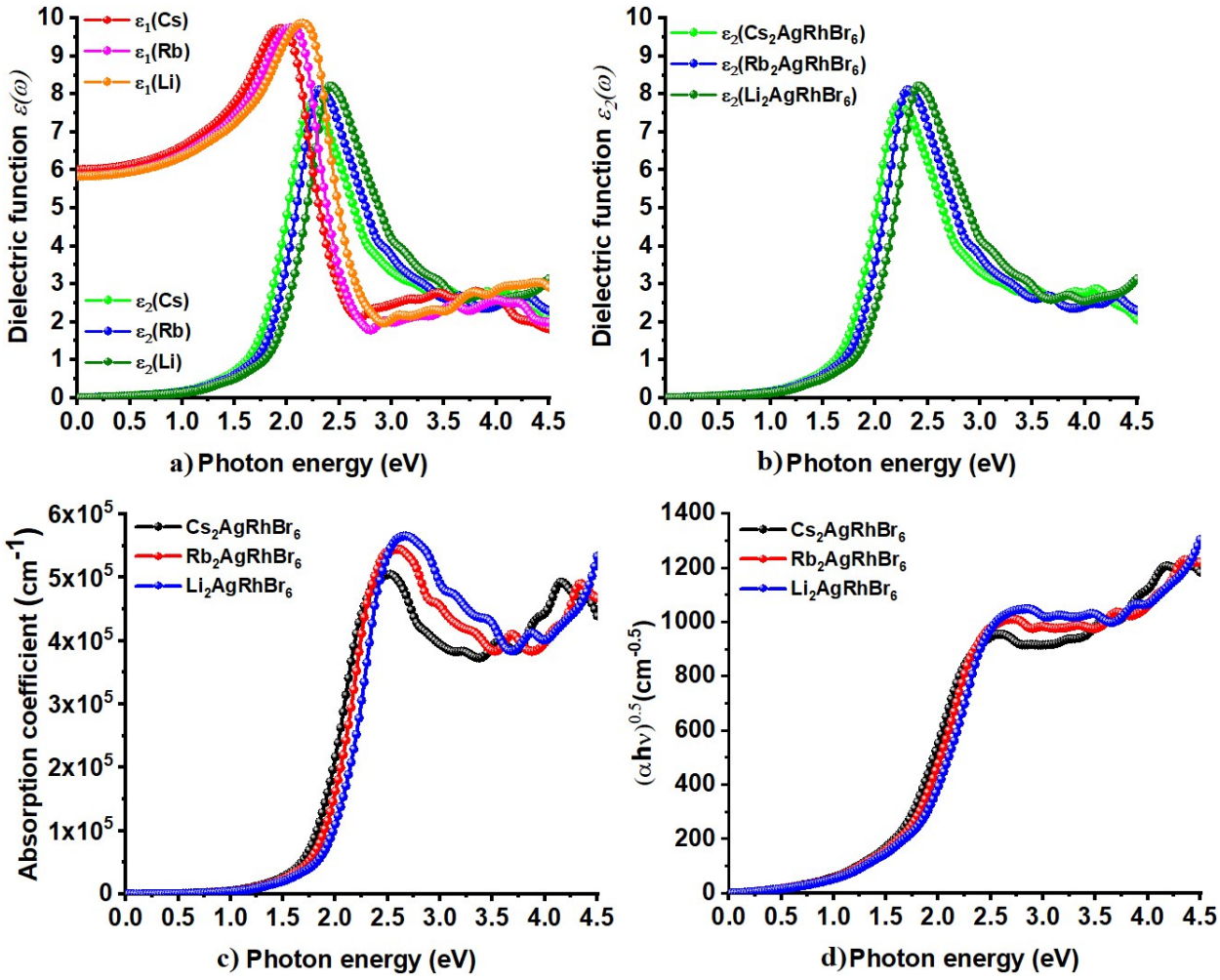

Figure S5: a) Dependence of SCAN-*rVV*10 computed real and imaginary parts of the dielectric function on the photon energy for $A_2AgRhBr_6$ (A = Cs, Rb, Li). b) Dependence of the imaginary part of the dielectric function on the photon energy for the corresponding systems; the plot is the same as that shown in a), but is repeated in b) for clarity. c) Dependence of absorption coefficient on the photon energy for the corresponding systems. d) The Tauc plot for the corresponding systems.

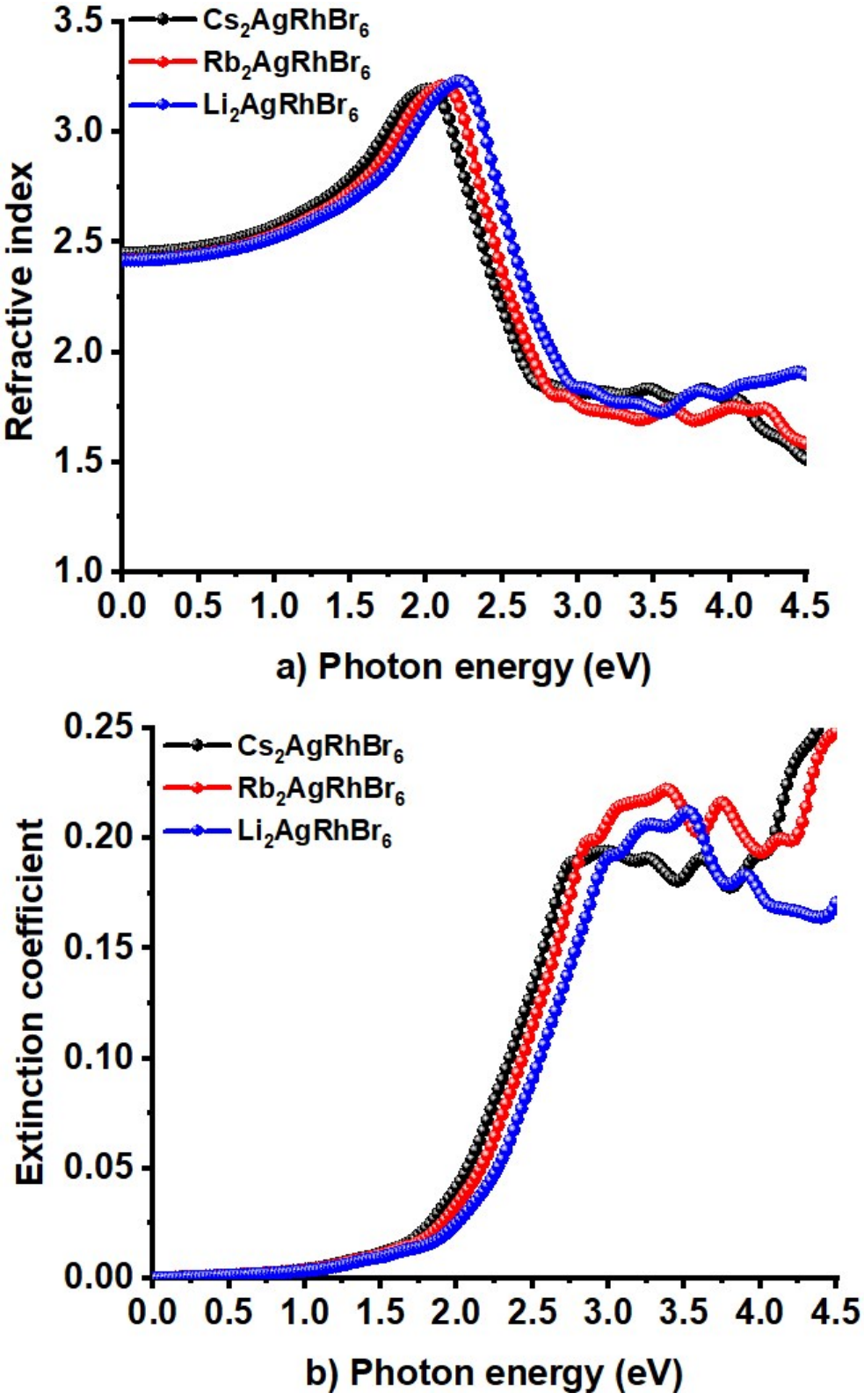

Figure S6: Dependence of SCAN-*rVV*10 computed a) real and b) imaginary parts of the refractive index on the photon energy for $A_2AgRhBr_6$ (A = Cs, Rb, Li).