Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information – First-principles study on elastic, electronic and optical properties of all-inorganic halide perovskite solid solutions $CsPb(Br_{1-x}Cl_x)_3$ within virtual crystal approximation

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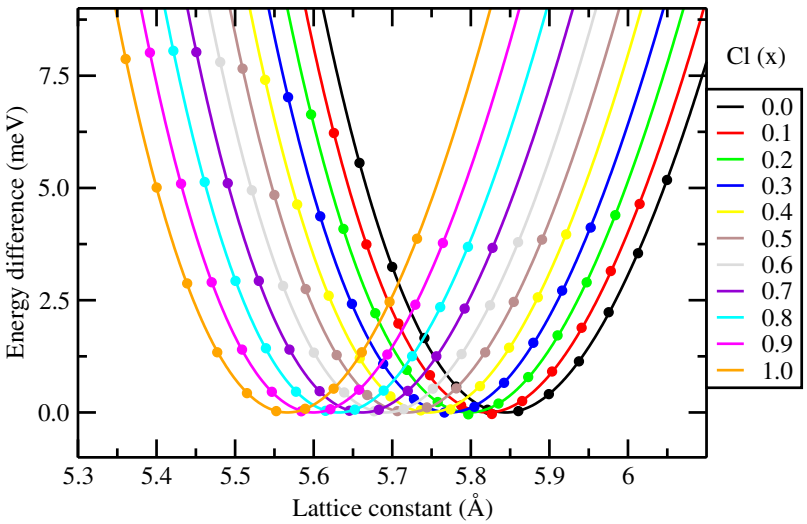

Figure S1. Energy–lattice constant curves obtained by fitting the calculation data into the natural strain equation of state (EOS) for crystalline solid solutions $CsPb(Br_{1-x}Cl_x)_3$ (x = [0, 1], interval 0.1).

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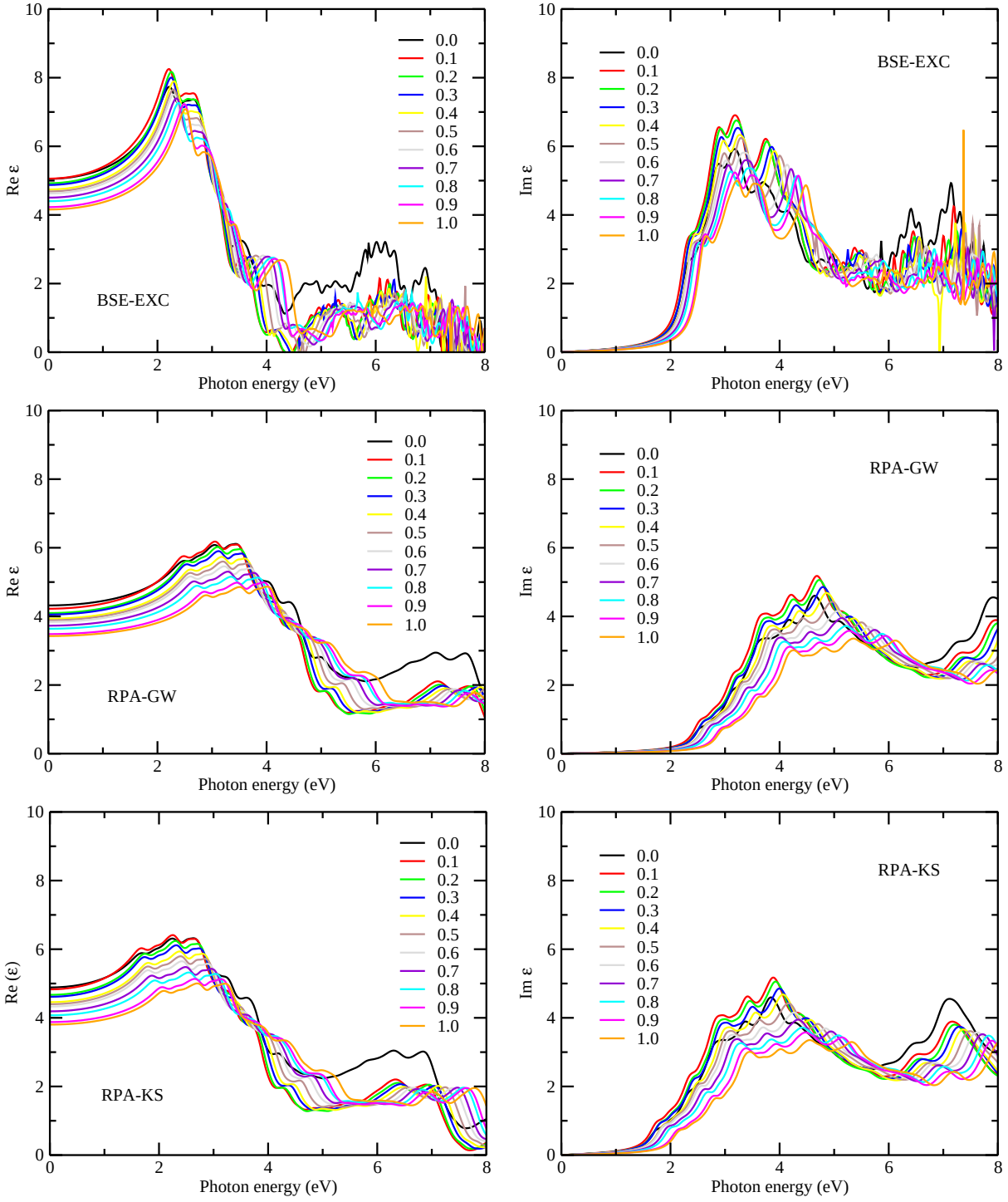

Figure S2. Frequency dependent dielectric constants of $CsPb(Br_{1-x}Cl_x)_3$ (x = [0, 1], interval 0.1), obtained by solving the Bethe-Salpeter equation with excitonic effect (BSE-EXC), *GW* equation within random phase approximation (RPA-*GW*) and Kohn-Sham equation with RPA (RPA-KS).

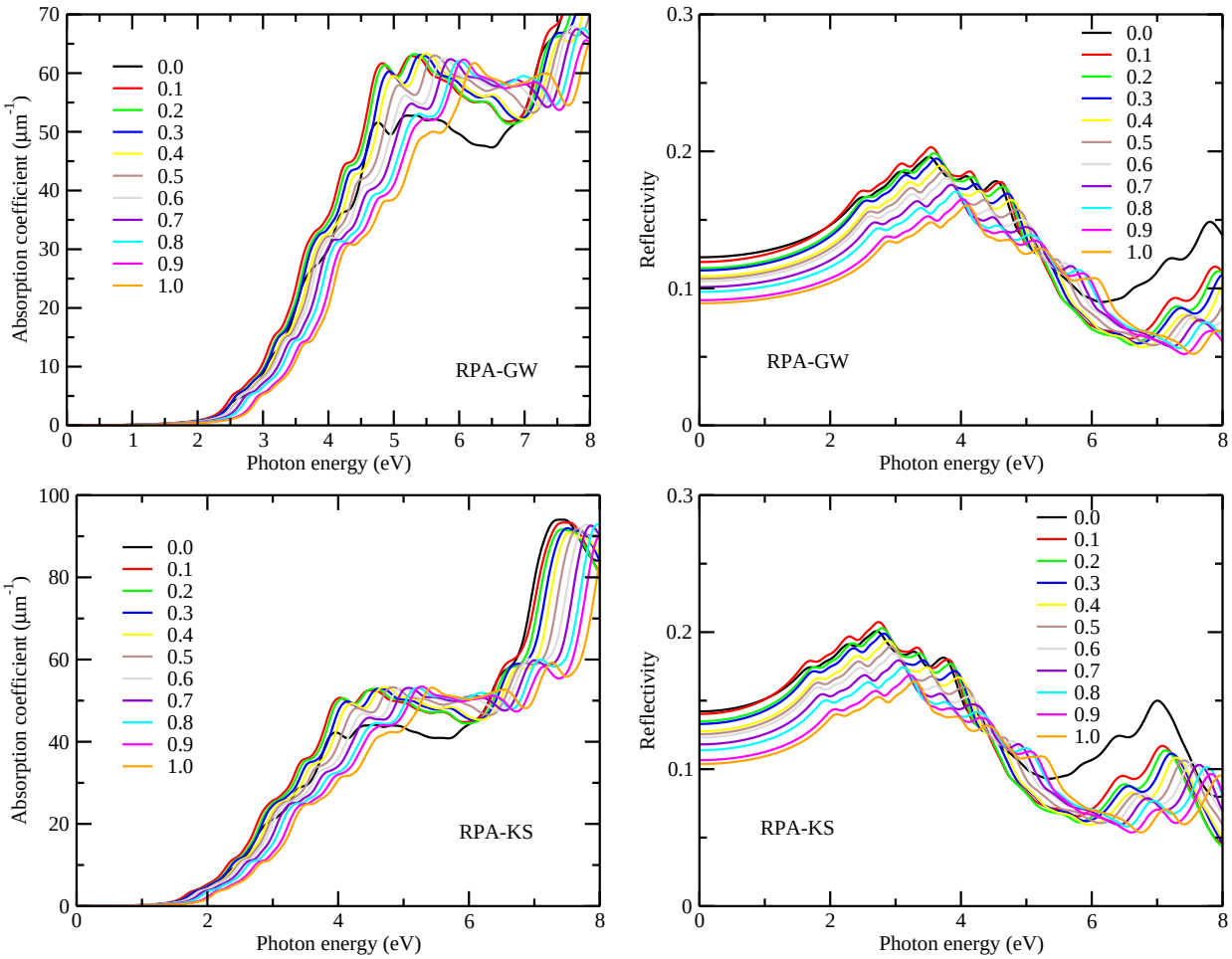

Figure S3. Photo-absorption coefficient (left panel) and reflectivity (right panel) of $CsPb(Br_{1-x}Cl_x)_3$ as a function of photon energy, obtained by using RPA-*GW* and RPA-KS approaches.

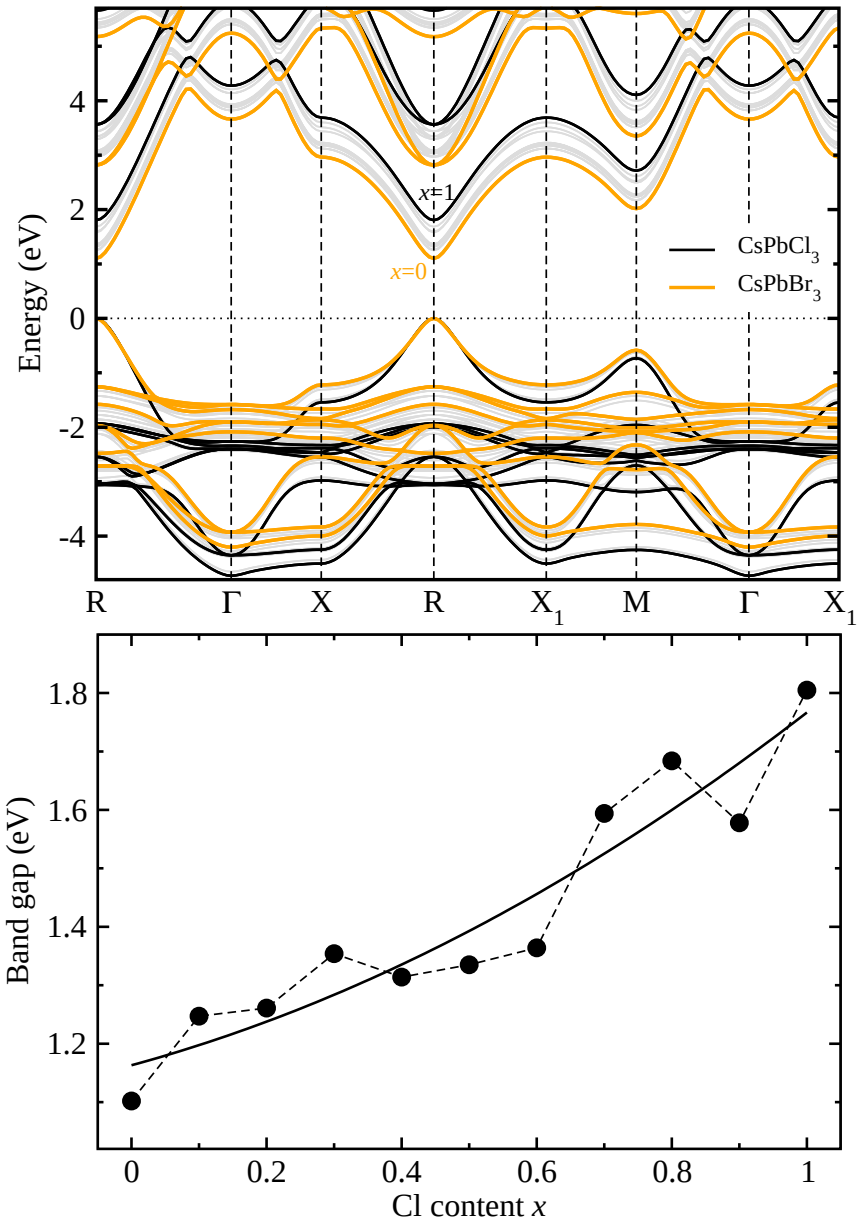

Figure S4. Band structures of cubic $CsPbX_3$ (X = $Br_{1-x}Cl_x$) (top) and band gaps (bottom) as increasing the Cl content x from 0 to 1, calculated with HSE06+SOC method. The band gap increases along the quadratic function of $E_g(x) = 1.163 + 0.316x + 0.288x^2$ (eV).

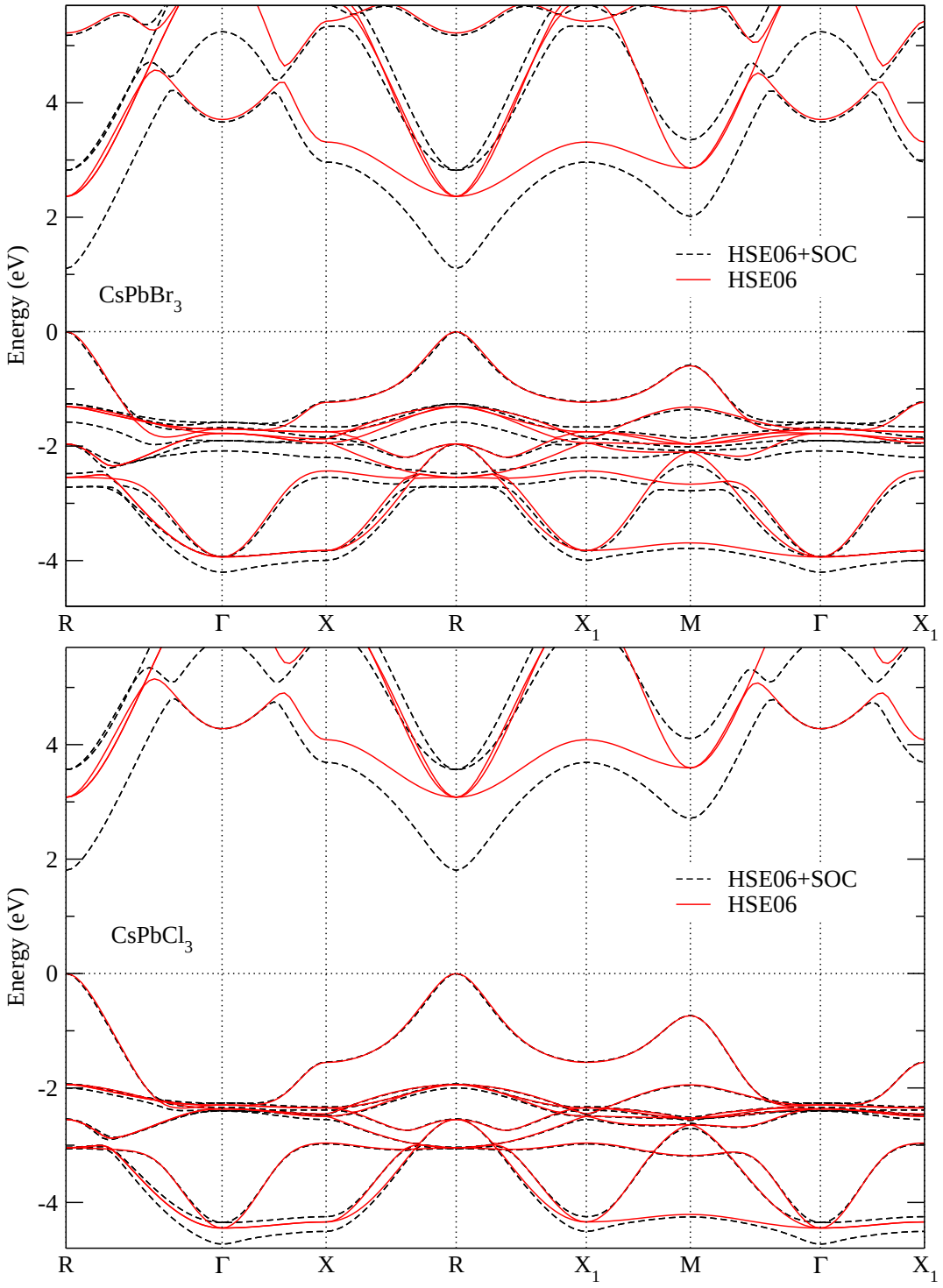

Figure S5. Comparison of band structures calculated with HSE06 (red solid line) and HSE06+SOC (black dashed line) for $CsPbBr_3$ (top) and $CsPbCl_3$ (bottom).