Electronic supplementary information

Computational study of the fundamental properties of Zr-based chalcogenide perovskites for optoelectronics

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Table 1S The calculated tolerance factor (t) values of $AZrX_3$ (A = Ca, Sr, Ba; X = S, Se). The ionic radii of various atoms are also provided.

Ionic	Ionic radius (Å)	Compound	t
Ca^{2+}	1.34	$CaZrS_3$	0.878
Sr^{2+}	1.58	$SrZrS_3$	0.945
Ba^{2+}	1.61	$BaZrS_3$	0.953
Zr^{4+}	0.72	$CaZrSe_3$	0.870
S^{2-}	1.84	$SrZrSe_3$	0.932
Se^{2-}	1.98	$BaZrSe_3$	0.940

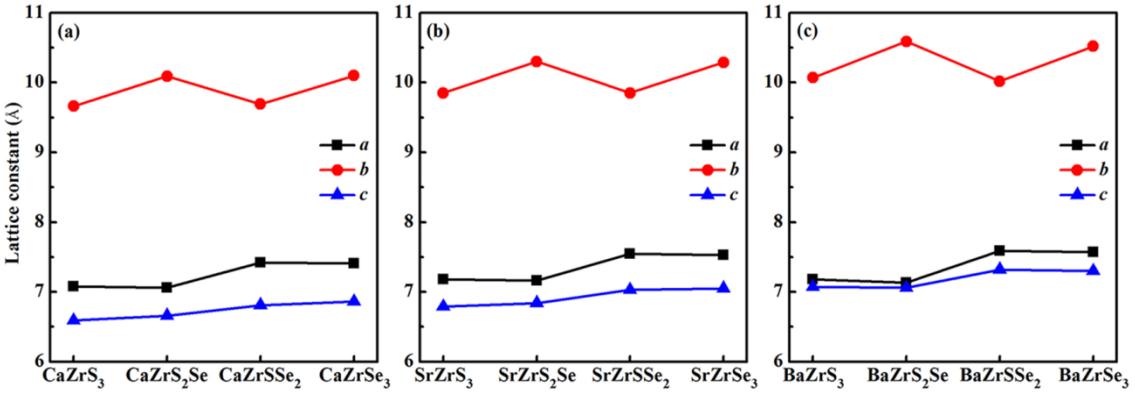

Fig. 1S The variation on the lattice constants of (a) $CaZrS_{3-x}Se_x$, (b) $SrZrS_{3-x}Se_x$, and (c) $BaZrS_{3-x}Se_x$ as a function of x.

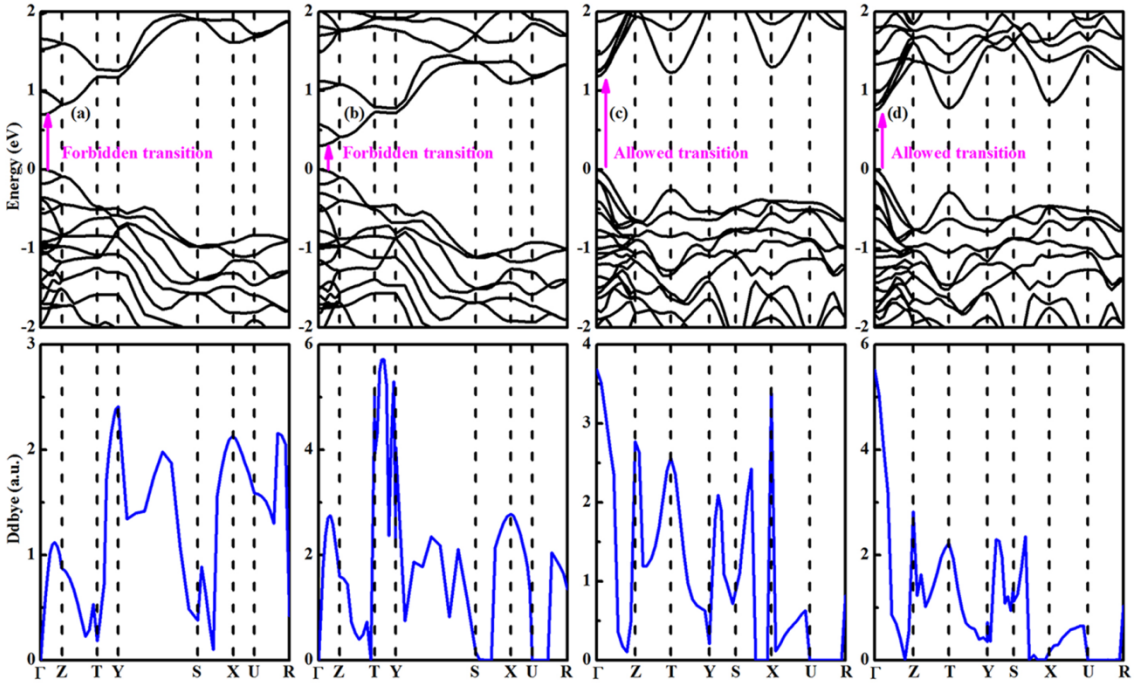

Fig. 2S The band structures (upper panels) and transition dipole moment (lower panels) of (a) α-$CaZrS_3$, (b) α-$CaZrSe_3$, (c) β-$CaZrS_3$, and (d) β-$CaZrSe_3$ at the PBE functional.