Supplementary information

High-throughput screening of transport behavior on tetragonal perovskite

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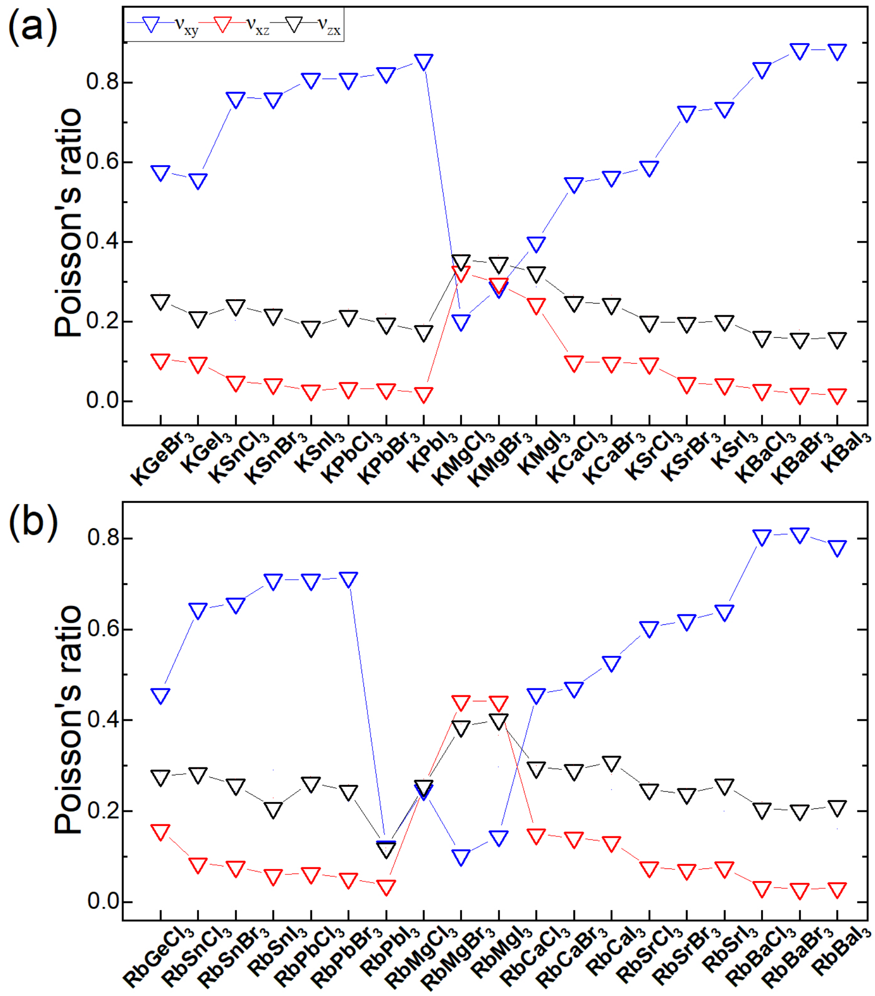

Figure S1. Poisson's ratio for K, Rb-based perovskites. (a) K-based perovskites, (b) Rb-based perovskites.

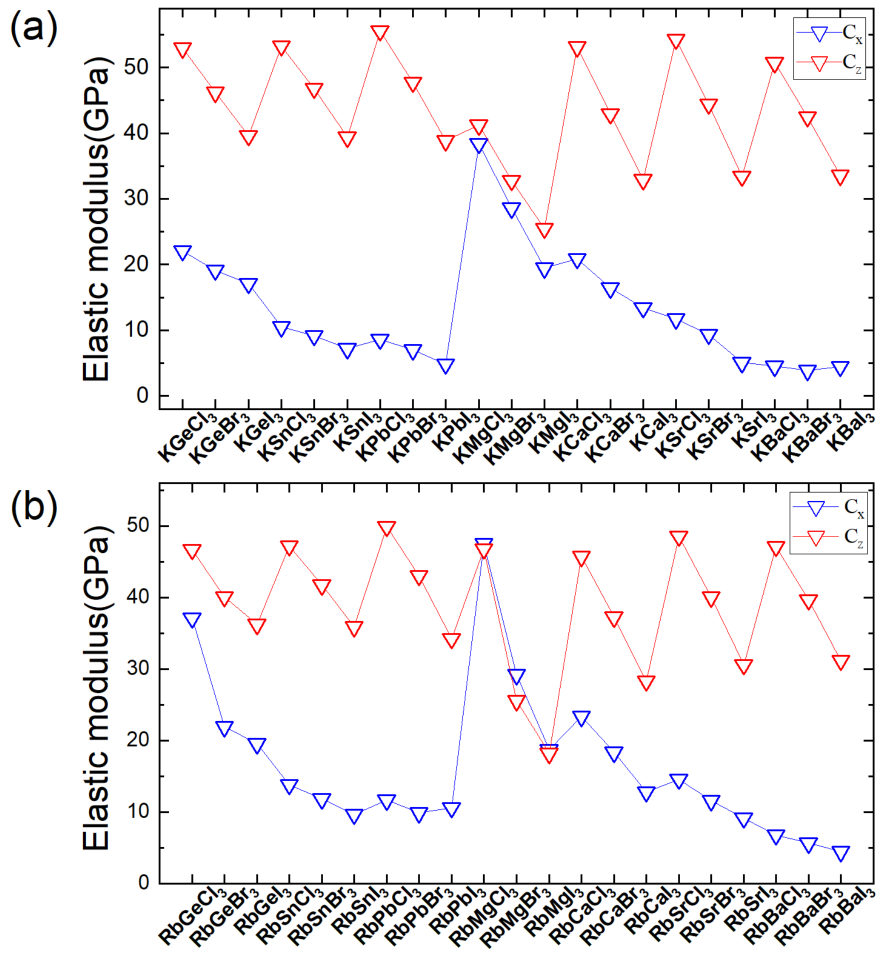

Figure S2. The elastic modulus for K, Rb-based perovskites. (a) K-based perovskites, (b) Rb-based perovskites.

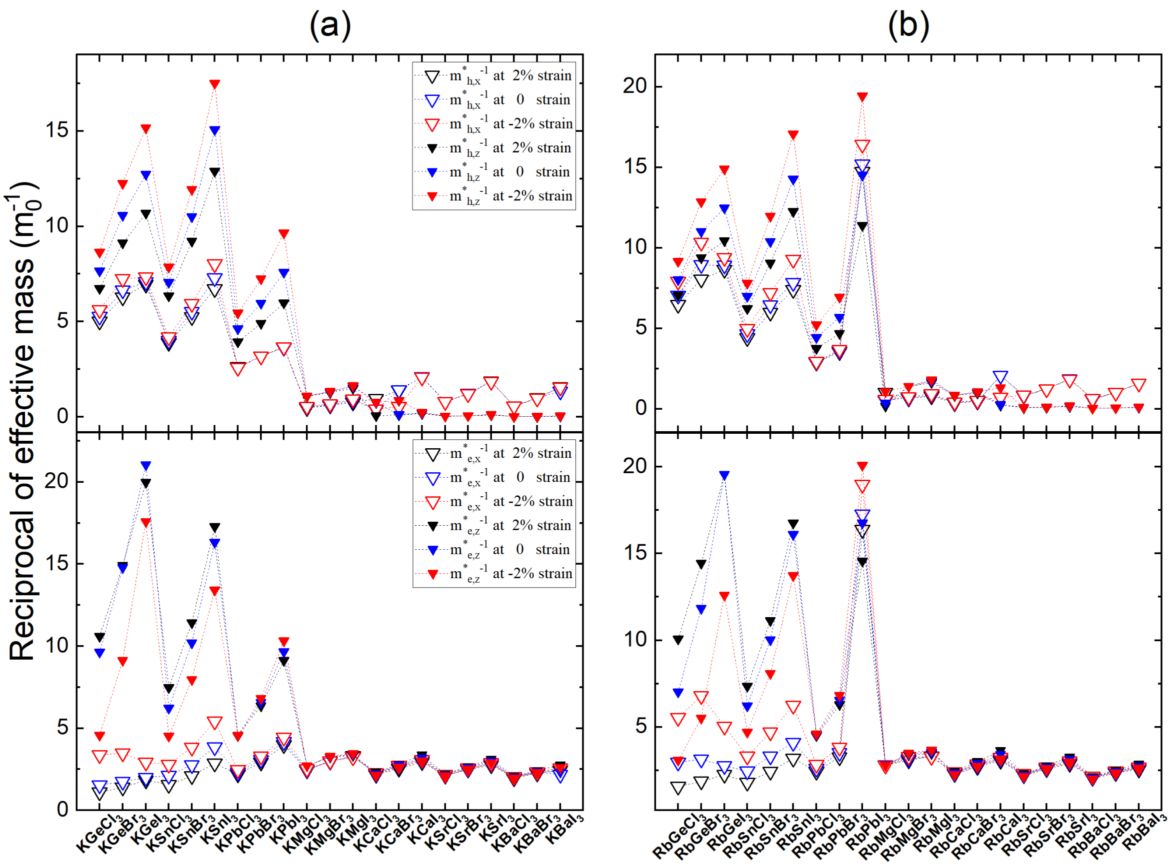

Figure S3. The reciprocal of effective mass for K, Rb-based perovskites. (a) K-based perovskites. (b) Rb-based perovskites.

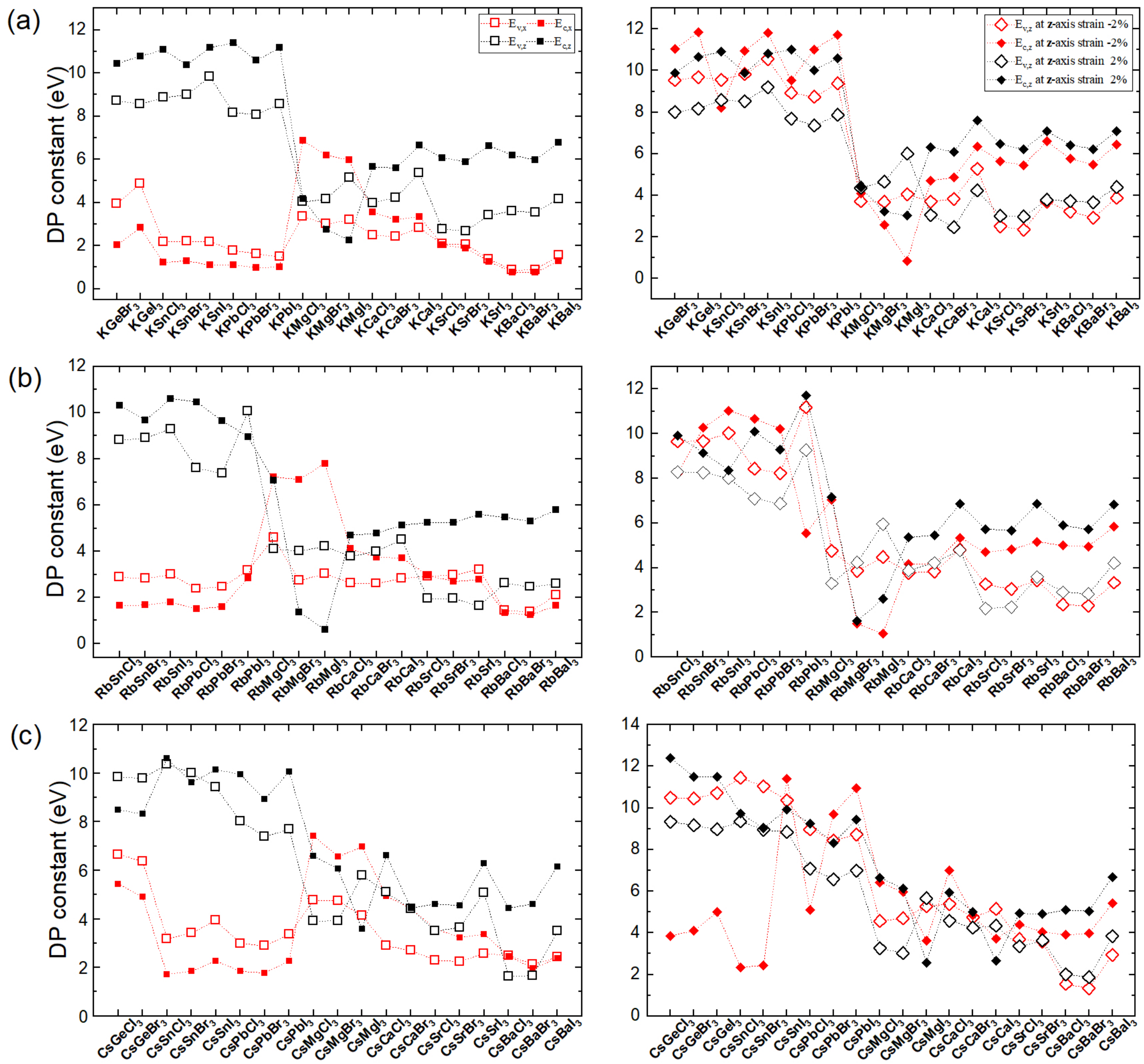

Figure S4. The deformation potential (DP) constant for K, Rb, Cs-based perovskites, which was obtained by the band edge shift at uniaxial strain. (a) K-based perovskites. (b) Rb-based perovskites. (c) Cs-based perovskites.

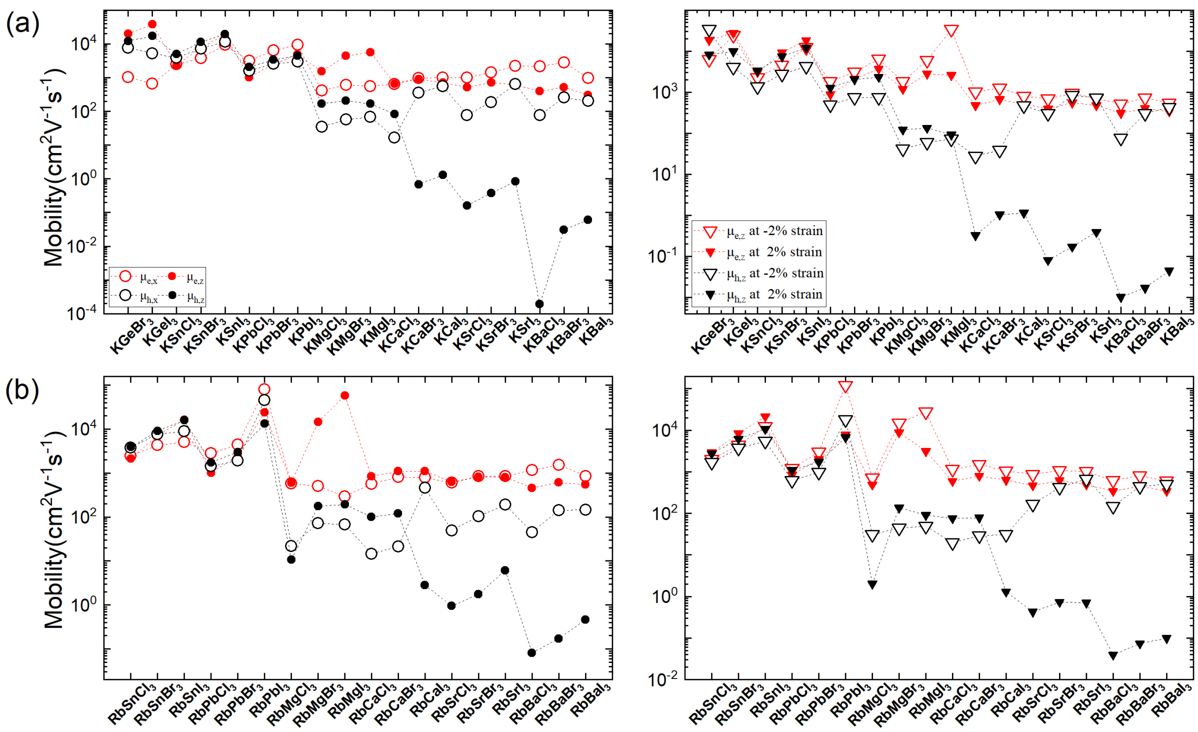

Figure S5. The electron and hole mobilities of K, Rb-based perovskites predicted by the LAP model. (a) K-based perovskites. (b) Rb-based perovskites.

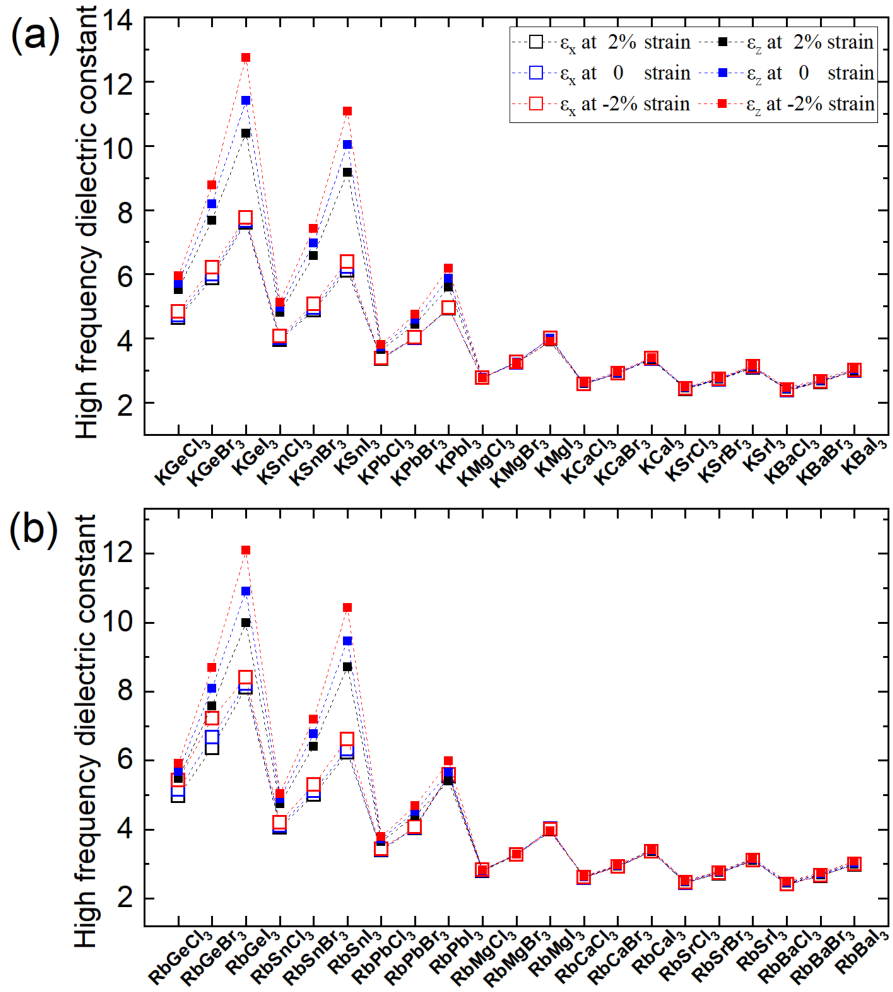

Figure S6. High frequency dielectric constants along x and z-axis directions for K, Rb-based perovskites. The results were calculated using fully relaxed lattice and z-axis strain of $\pm 2\%$.

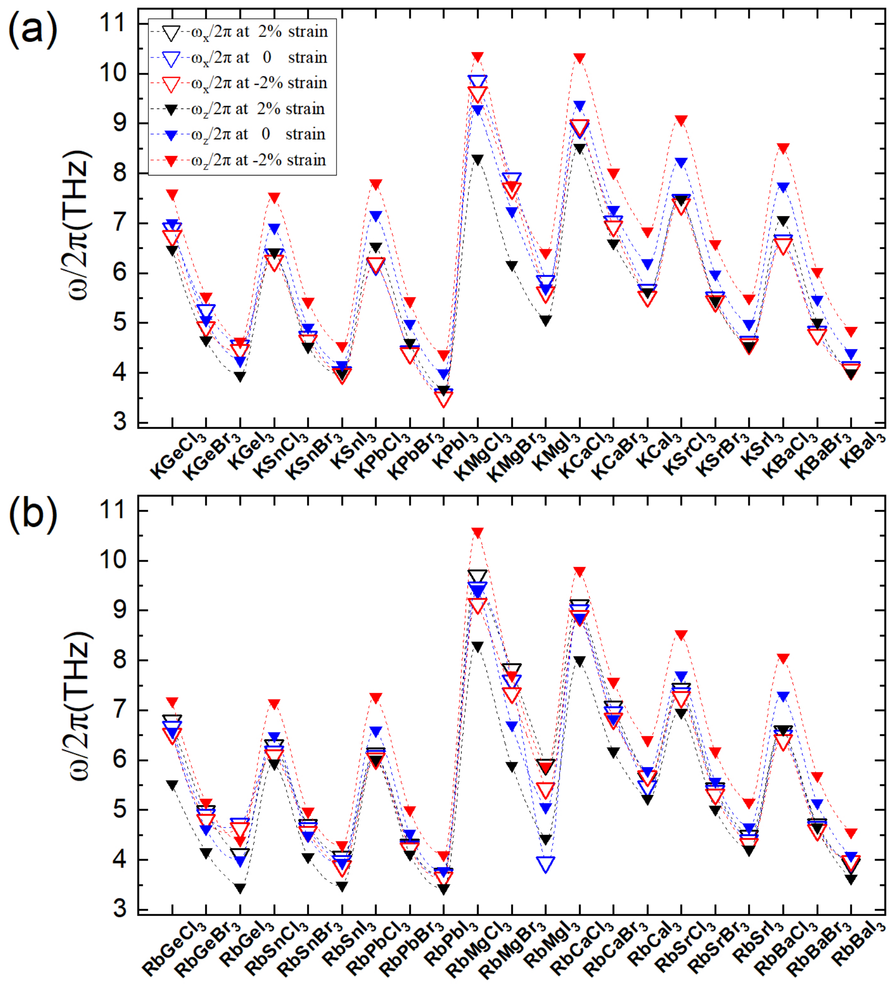

Figure S7. The longitudinal optical phonon frequency of K, Cs-based perovskites. The results were calculated using fully relaxed lattice and z-axis strain of $\pm2\%$.

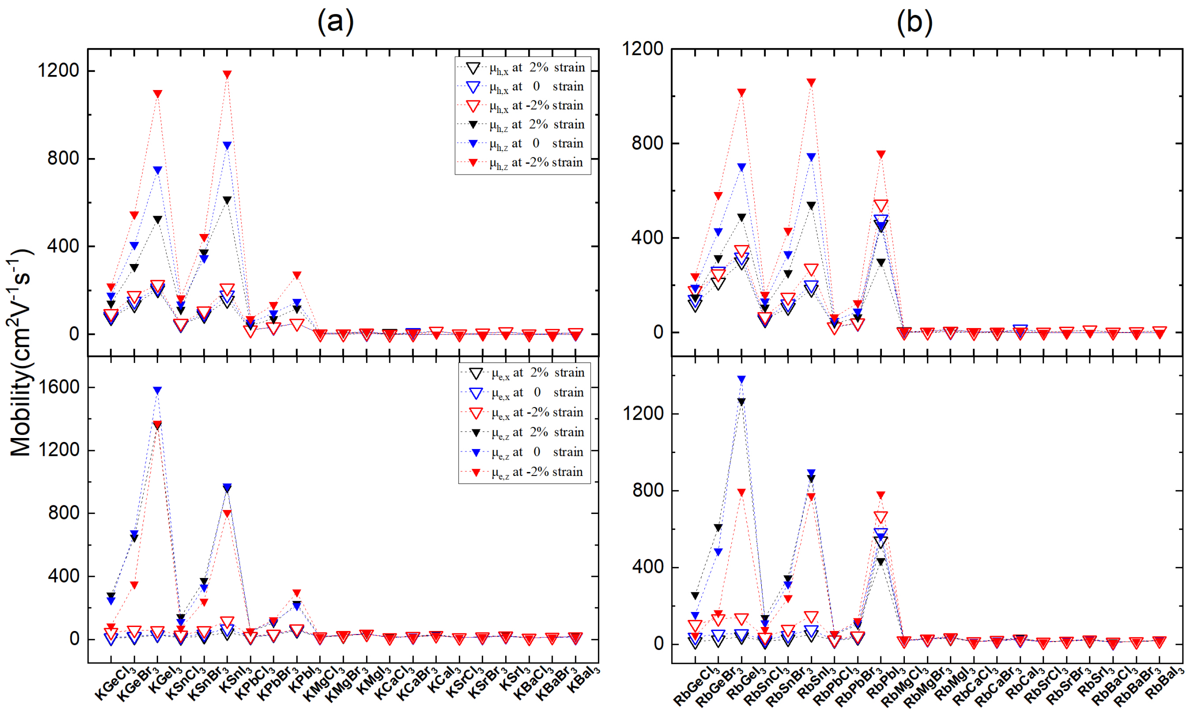

Figure S8. The mobility of K, Rb-based perovskites was predicted by the POP model. (a) K-based perovskites, (b) Rb-based perovskites.

Table S1. Under the compressive strain of -4%, some perovskites were predicted to exhibit high carrier mobility.

Material	a/c(Å)	$\mu_{e,x}$($cm^2V^{-1}s^{-1}$)	$\mu_{e,z}$($cm^2V^{-1}s^{-1}$)	$\mu_{h,x}$($cm^2V^{-1}s^{-1}$)	$\mu_{h,z}$($cm^2V^{-1}s^{-1}$)
$CsGeBr_3$	7.99/5.38	533	69	811	764
$CsGeI_3$	8.53/5.78	1070	211	1334	1665
$CsSnI_3$	8.87/6.10	960	814	1268	2013
$KGeI_3$	8.31/5.76	197	392	261	1643
$KSnI_3$	8.67/6.03	205	605	280	1659
$RbGeBr_3$	7.89/5.39	376	83	568	809
$RbGeI_3$	8.42/5.80	514	242	612	1555
$RbSnI_3$	8.74/6.08	303	637	415	1560