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Supplementary Information for

Strain-induced bandgap engineering in $CsGeX_3$ (X = I, Br or Cl) perovskites: Insights from first-principle calculations

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Supplementary Table 1. Theoretical and experimental values of lattice parameter a (Å) and unit cell volume V (Å^3) of $CsGeX_3$ perovskites.

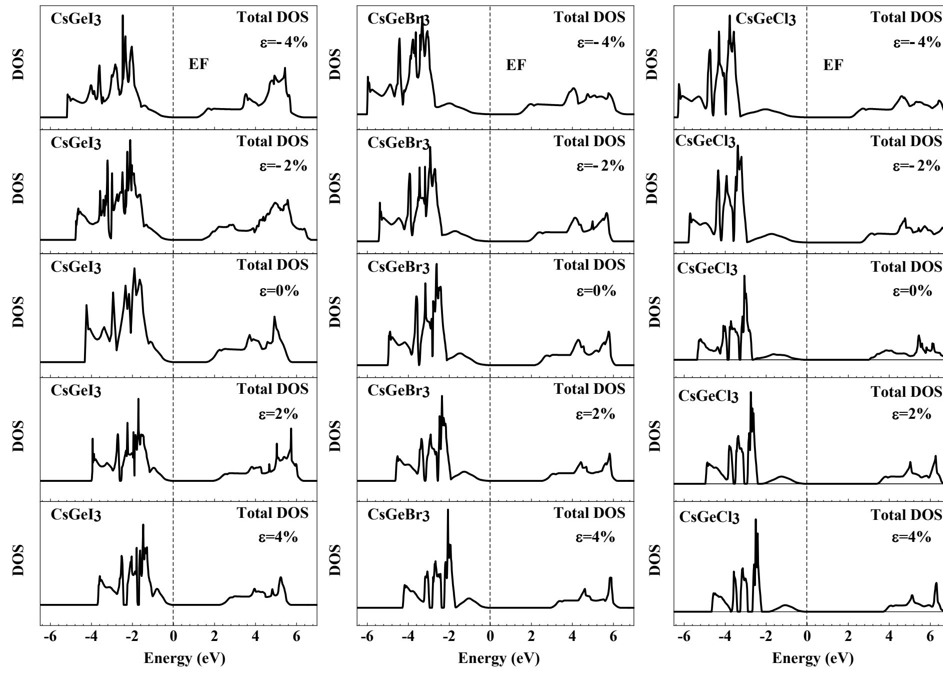
	a (Å)			V (Å^3)
	This Work	Other Works	Experimental	
$CsGeI_3$	5.92	5.99[1]	5.983[1]	233.8
$CsGeBr_3$	5.76	5.36[2], 5.64[3], 5.69[1]	5.636[1], 5.362[4]	191.6
$CsGeCl_3$	5.53	5.43[3], 5.52[5], 5.51[1]	5.434[1]	168.9

Supplementary Table 2. Calculated electronic bandgaps (in eV), some available theoretical results and experimental optical bandgaps (in eV) of perovskites $CsGeX_3$ (X=I, Br or Cl).

Phase	This Work	Other Works	Expt.
$CsGeI_3$	1.6	1.02[1], 1.17 (PBE)[6], 1.48 (HSE)[6]	1.53[1]
$CsGeBr_3$	2.13	0.55 (PBE)[2], 4.74 (EHTB)[3], 1.49[1], 1.48 (PBE) [6], 1.97 (HSE)[6]	2.32[1]
$CsGeCl_3$	2.99	7.91 (EHTB)[3], 2.11 (PBE)[5], 0.82 (PBE)[7], 2.26[1], 2.17 (PBE)[6], 2.48 (HSE)[6]	3.31[8]

Supplementary Table 3. Bandgaps (in eV) of $CsGeX_3$ (X=I, Br or Cl) under the triaxial strains from −4% to 4%.

Strain / phase	−4%	−3%	−2%	−1%	0	1%	2%	3%	4%
$CsGeI_3$	1.05	1.23	1.35	1.48	1.61	1.75	1.89	2.02	2.21
$CsGeBr_3$	1.26	1.53	1.75	1.93	2.13	2.32	2.49	2.64	2.90
$CsGeCl_3$	2.05	2.33	2.57	2.80	3.00	3.20	3.37	3.54	3.68



Supplementary Figure 1: Total densities of states of $CsGeX_3$ (X=I, Br or Cl) perovskites under different strains.

Supplementary Table 4. Effective masses of electron and hole of $CsGeI_3$, $CsGeBr_3$, and $CsGeCl_3$ under the strains.

directions / strains	electrons			holes		
	R→Γ(m_0)	R→M(m_0)	R→X(m_0)	R→Γ(m_0)	R→M (m_0)	R→X (m_0)
−4% ($CsGeI_3$)	0.129	0.898	0.650	0.131	0.263	0.168
−3%($CsGeI_3$)	0.138	0.843	0.450	0.142	0.271	0.180
−2%($CsGeI_3$)	0.148	0.781	0.342	0.153	0.276	0.191
−1%($CsGeI_3$)	0.162	0.648	0.309	0.170	0.297	0.211
0%($CsGeI_3$)	0.176	0.633	0.310	0.186	0.327	0.233
1%($CsGeI_3$)	0.197	0.512	0.298	0.212	0.349	0.259
2%($CsGeI_3$)	0.218	0.490	0.307	0.239	0.384	0.291
3%($CsGeI_3$)	0.240	0.483	0.321	0.270	0.426	0.326
4%($CsGeI_3$)	0.266	0.478	0.337	0.318	0.488	0.381
−4%($CsGeBr_3$)	0.115	1.184	1.271	0.112	0.165	0.134
−3%($CsGeBr_3$)	0.138	1.070	0.640	0.138	0.183	0.152
−2%($CsGeBr_3$)	0.157	0.791	0.410	0.159	0.208	0.175
−1%($CsGeBr_3$)	0.178	0.614	0.330	0.181	0.236	0.200
0%($CsGeBr_3$)	0.191	0.561	0.315	0.197	0.256	0.218
1%($CsGeBr_3$)	0.227	0.548	0.332	0.237	0.305	0.262
2%($CsGeBr_3$)	0.254	0.537	0.345	0.269	0.344	0.297
3%($CsGeBr_3$)	0.280	0.528	0.364	0.302	0.386	0.334
4%($CsGeBr_3$)	0.316	0.522	0.421	0.357	0.453	0.394
−4%($CsGeCl_3$)	0.361	1.025	0.931	0.183	0.217	0.194
−3%($CsGeCl_3$)	0.380	1.053	1.007	0.210	0.250	0.224
−2%($CsGeCl_3$)	0.404	1.109	1.113	0.239	0.283	0.254
−1%($CsGeCl_3$)	0.421	1.143	1.207	0.270	0.318	0.286
0%($CsGeCl_3$)	0.450	1.191	1.092	0.300	0.354	0.320
1%($CsGeCl_3$)	0.487	1.204	1.327	0.333	0.393	0.355
2%($CsGeCl_3$)	0.488	1.237	1.085	0.385	0.454	0.411
3%($CsGeCl_3$)	0.514	1.289	1.068	0.426	0.501	0.455
4%($CsGeCl_3$)	0.537	1.335	1.119	0.472	0.557	0.507

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