

Supporting Information

**High-throughput calculation for screening of For
mamidinium Halide Perovskite for Solar Cells**

Tomoya Tashiro†, Hajime Suzuki† and Keisuke Takahashi†*

†Department of Chemistry, Hokkaido University, North 10, West 8, Sapporo 060-8510, Japan

*Corresponding Author:

E-mail: tt_hokudai7613@eis.hokudai.ac.jp; keisuke.takahashi@sci.hokudai.ac.jp

configuration	Energy	lattice_constant	Total_magnetic_moment	Eks(PBEsol)	Dxc	Eks+Dxc(GLLB-sc)	formation E	Tolerance Factor	Latticedistortion
FAGeFFF	-65.9525	5.991047111	0	4.57215895	1.925091	6.497250311	-0.92239155	1.170323 >1	26.8282 >15%
FAGeFFCI	-64.5513	5.991047111	0	4.25484617	1.726425	5.981270745	-0.82015789	1.133308 >1	18.70276 >15%
FAGeFFBr	-64.1086	6.043370667	0	3.80716072	1.521043	5.328203259	-0.80724549	1.123795 >1	19.96732 >15%
FAGeFFI	-63.6683	6.043370667	0	2.62816631	0.99674	3.624906254	-0.78655595	1.109426 >1	17.71656 >15%
FAGeFCIF	-63.0576	6.043370667	0	did not converge in band calc			-0.69568733	1.133308 >1	12.31528
FAGeFCICI	-62.4702	6.043370667	0	3.45413975	1.418452	4.872591682	-0.66127109	1.101771 >1	20.44091 >15%
FAGeFCIBr	-62.1554	6.043370667	0	3.08983128	1.258273	4.348104408	-0.65901786	1.0936 >1	14.91361
FAGeFCII	-61.8697	6.095694222	0	2.23861305	0.874577	3.113190083	-0.651212	1.081207 >1	13.57603
FAGeFBrF	-62.5292	6.043370667	0	3.71564004	1.654109	5.369748676	-0.67563057	1.123795 >1	14.33071
FAGeFBrCl	-61.9236	6.043370667	0	3.17266647	1.328219	4.500885166	-0.63969728	1.0936 >1	17.4831 >15%
FAGeFBrBr	-61.7318	6.095694222	0	2.76578753	1.13788	3.90366772	-0.64768985	1.08576 >1	11.39663
FAGeFBrI	-61.3271	6.095694222	0	2.15716497	0.860867	3.018032391	-0.6299709	1.073858 >1	11.68735
FAGeFIIF	-61.8875	6.095694222	0	2.79367881	1.186026	3.97970504	-0.63815628	1.109426 >1	11.64653
FAGeFICI	-61.4079	6.095694222	0	2.35378268	0.940285	3.294068178	-0.61272732	1.081207 >1	14.68406
FAGeFIBr	-61.1615	6.095694222	0	2.14475964	0.851585	2.996344238	-0.61616572	1.073858 >1	10.617
FAGeFII	-60.8165	6.095694222	0	1.66932986	0.662672	2.332001692	-0.60342167	1.06268 >1	13.16293
FAGeCIFF	-63.1223	6.043370667	0	4.02616338	1.718897	5.745060656	-0.70107379	1.133308 >1	17.52322 >15%
FAGeCIFCI	-62.5715	6.043370667	0	3.51784397	1.428874	4.946717695	-0.66971217	1.101771 >1	17.2934 >15%
FAGeCIFBr	-62.2895	6.043370667	0	3.07962331	1.232042	4.31166487	-0.67018874	1.0936 >1	17.39117 >15%
FAGeCIFI	-61.8514	6.095694222	0	2.27298509	0.888944	3.161929112	-0.64968232	1.081207 >1	17.89879 >15%
FAGeCICIF	-61.1191	6.043370667	0	3.63714547	1.597526	5.234671696	-0.54868058	1.101771 >1	10.78679
FAGeCICICI	-60.5295	6.148017778	0	3.07225628	1.297442	4.369698115	-0.51408833	1.07458 >1	12.30014
FAGeCICIBr	-60.1535	6.148017778	0	2.59773575	1.084041	3.681776252	-0.50672502	1.067486 >1	10.40902
FAGeCICII	-59.8498	6.148017778	0	1.97778079	0.80241	2.780191147	-0.49742604	1.056688 >1	10.65554
FAGeCIBrF	-60.5103	6.095694222	0	3.2957087	1.46443	4.76013833	-0.52192102	1.0936 >1	8.453156
FAGeCIBrCl	-59.8873	6.148017778	0	2.83430529	1.215323	4.049628545	-0.48453988	1.067486 >1	8.884469
FAGeCIBrBr	-59.6623	6.148017778	0	2.47504549	1.050252	3.525297121	-0.48976429	1.06066 >1	8.944563
FAGeCIBrI	-59.3595	6.148017778	0	1.8473628	0.758527	2.605889964	-0.48053631	1.050262 >1	8.050828
FAGeCIIF	-59.9397	6.095694222	0	2.55688792	1.172459	3.729347295	-0.49037783	1.081207 >1	12.88515
FAGeCIICI	-59.3267	6.148017778	0	2.25294961	0.993215	3.246164707	-0.45383086	1.056688 >1	10.31684
FAGeCIIBr	-59.0983	6.148017778	0	1.95164227	0.850881	2.802523747	-0.45876915	1.050262 >1	9.741946
FAGeCIII	-58.8206	6.148017778	0	1.54997036	0.656542	2.206511897	-0.45163295	1.040457 >1	8.966114
FAGeBrFF	-62.6307	6.043370667	0	3.65168353	1.558246	5.209929382	-0.68408615	1.123795 >1	18.20963 >15%
FAGeBrFCI	-62.1233	6.043370667	0	3.24311943	1.321268	4.564387911	-0.65633864	1.0936 >1	17.2265 >15%
FAGeBrFBr	-61.5973	6.095694222	0	2.88108794	1.18271	4.063798341	-0.63647952	1.08576 >1	17.5389 >15%
FAGeBrFI	-61.3994	6.095694222	0	2.11260519	0.834046	2.946650688	-0.63599024	1.073858 >1	17.37671 >15%
FAGeBrCIF	-60.5715	6.095694222	0	did not converge in band calc			-0.5270204	1.0936 >1	12.8963
FAGeBrCICI	-59.8887	6.148017778	0	2.8086692	1.197053	4.005722225	-0.48465945	1.067486 >1	10.11289
FAGeBrClBr	-59.7197	6.148017778	0	2.54627509	1.074339	3.620614237	-0.49455331	1.06066 >1	10.98962
FAGeBrCII	-59.3556	6.148017778	0	1.81714204	0.744174	2.561316098	-0.48021303	1.050262 >1	9.038073
FAGeBrBrF	-60.0017	6.095694222	0	3.05180768	1.365302	4.417109705	-0.50351028	1.08576 >1	8.141378
FAGeBrBrCl	-59.3824	6.148017778	0	2.67521175	1.160439	3.835650247	-0.46644104	1.06066 >1	8.423892
FAGeBrBrBr	-59.1531	6.148017778	0	2.26339613	0.968256	3.231652603	-0.47131203	1.054089 >1	7.871692
FAGeBrBrI	-58.8671	6.148017778	0	1.73417435	0.720505	2.454678856	-0.46348054	1.044067 >1	7.316191
FAGeBrIF	-59.4299	6.095694222	0	2.4121263	1.119997	3.532123643	-0.47186636	1.073858 >1	9.995035
FAGeBrICI	-58.8092	6.148017778	0	2.10465092	0.938133	3.042784411	-0.43468219	1.050262 >1	8.265333
FAGeBrIBr	-58.5925	6.148017778	0	1.82903225	0.80926	2.638292308	-0.44059316	1.044067 >1	7.406314
FAGeBrIII	-58.2924	6.200341333	0	1.52909311	0.661881	2.190973931	-0.4315966	1.034609 >1	7.045773
FAGelFF	-62.6361	6.095694222	0	2.6525085	1.163379	3.81588752	-0.7005368	1.109426 >1	20.04695 >15%
FAGelFCI	-61.5795	6.095694222	0	2.468717	1.01828	3.486996557	-0.62702449	1.081207 >1	18.98631 >15%
FAGelFBr	-61.266	6.095694222	0	2.2041841	0.904133	3.10831691	-0.62487257	1.073858 >1	17.31838 >15%
FAGelFI	-60.8632	6.095694222	0	1.69661278	0.68013	2.376742442	-0.59130695	1.06268 >1	14.26956
FAGelCIF	-59.9795	6.095694222	0	2.56332672	1.135565	3.698976702	-0.49369058	1.081207 >1	12.36022
FAGelCICI	-59.4583	6.148017778	0	2.30160917	0.98622	3.287829297	-0.46479497	1.056688 >1	12.23838
FAGelCIBr	-59.1064	6.148017778	0	1.90452228	0.814701	2.719223743	-0.4594517	1.050262 >1	8.533982
FAGelCII	-58.8182	6.148017778	0	1.49446809	0.625122	2.119589732	-0.45143945	1.040457 >1	7.941962
FAGelBrF	-59.417	6.095694222	0	2.41739584	1.096622	3.514017946	-0.47079112	1.073858 >1	7.293733
FAGelBrCl	-58.8107	6.148017778	0	2.09444866	0.917529	3.011977524	-0.43480516	1.050262 >1	6.977545
FAGelBrBr	-58.5972	6.148017778	0	1.8213582	0.793425	2.614783005	-0.44098946	1.044067 >1	6.822117
FAGelBrI	-58.3018	6.200341333	0	1.51775647	0.650702	2.168458496	-0.43237971	1.034609 >1	6.479649
FAGelIF	-58.6574	6.200341333	0	2.16183178	1.035883	3.197714701	-0.42349771	1.06268 >1	7.362096
FAGelICI	-58.194	6.200341333	0	1.80949119	0.830511	2.64000246	-0.39942003	1.040457 >1	5.750087
FAGelIBr	-57.9977	6.200341333	0	1.58733304	0.725678	2.313011061	-0.40703943	1.034609 >1	5.747486
FAGelIII	-57.7545	6.200341333	0	1.29667869	0.576427	1.873105843	-0.40277381	1.025667 >1	5.778904

Table S1 All data of Ge-Based Compositions.

configuration	Energy	lattice_constant	Total_magnetic_moment	Eks(PBEsol)	Dxc	Eks+Dxc(GLLB-sc)	formation E	Tolerance Factor	Latticedistortion
FASnFFF							did not converge in relax		
FASnFFCI							did not converge in relax		
FASnFFBr							did not converge in relax		
FASnFFI	-63.3397	6.095694222	0	2.796484985	0.897833	3.694318439	-0.7991013	1.021376 >1	17.70666 >15%
FASnFCIF	-63.3313	6.043370667	0	3.904005899	1.72611	5.630115677	-0.7584195	1.038471 >1	11.10101
FASnFCICI	-62.4809	6.095694222	0	3.179275179	1.341551	4.520826216	-0.7020885	1.015863 >1	14.54062
FASnFCIBr	-62.2177	6.095694222	0	2.663128364	1.085993	3.749120961	-0.7041308	1.009959 >1	11.07474
FASnFCII	-61.7941	6.095694222	0	2.214570109	0.867329	3.08189928	-0.6848337	1.000969 >1	13.99517
FASnFBrF	-62.8465	6.095694222	0	3.422162213	1.404252	4.826413753	-0.7419928	1.03168 >1	11.03922
FASnFBrCl	-62.1156	6.095694222	0	2.707082494	1.084594	3.791676099	-0.6956188	1.009959 >1	10.73873
FASnFBrBr	-61.8556	6.095694222	0	2.295744709	0.914879	3.2106238	-0.6979273	1.004277 >1	11.87268
FASnFBrI	-61.3439	6.095694222	0	1.538847584	0.606329	2.145177056	-0.6712896	0.995617	11.19328
FASnFIF	-62.0876	6.095694222	0	2.211521637	0.921528	3.133050004	-0.6947546	1.021376 >1	6.539767
FASnFICI	-61.3316	6.200341333	0	2.142139404	0.864688	3.006827088	-0.6462979	1.000969 >1	10.76809
FASnFIBr	-61.0647	6.200341333	0	1.897304447	0.807632	2.704936405	-0.6480268	0.995617	11.98395
FASnFI	-60.6377	6.252664889	0	1.412748115	0.564465	1.977213512	-0.6284519	0.987446	9.649109
FASnCIFF	-63.711	6.043370667	0	3.748583149	1.711437	5.460020496	-0.7900591	1.038471 >1	28.60511 >15%
FASnCIFFCI	-62.6795	6.095694222	0	3.221860508	1.328156	4.550016499	-0.7186434	1.015863 >1	17.74063 >15%
FASnCIFBr	-62.3706	6.095694222	0	2.843004523	1.150968	3.993972496	-0.7168684	1.009959 >1	17.70107 >15%
FASnCIF	-61.8988	6.095694222	0	2.758550698	1.098625	3.857175939	-0.6935599	1.000969 >1	18.01852 >15%
FASnCIFFCI	-61.4775	6.095694222	0	3.359486333	1.506792	4.866278009	-0.6184714	1.015863 >1	11.45173
FASnCIFFCI	-60.8377	6.148017778	0	2.837594395	1.208626	4.046220797	-0.5796905	0.996143	15.1265 >15%
FASnCIFFBr	-60.5246	6.148017778	0	2.443767832	1.024268	3.468036229	-0.5775769	0.990963	15.10767 >15%
FASnCIFFI	-60.052	6.200341333	0	1.805152304	0.734284	2.539436636	-0.5541945	0.983051	14.20163
FASnCIFFBr	-60.9064	6.095694222	0	2.689304102	1.114878	3.804182079	-0.5948568	1.009959 >1	5.495062
FASnCIFFCl	-60.2371	6.148017778	0	2.512334349	1.082382	3.594716506	-0.5536149	0.990963	7.570508
FASnCIFFBr	-59.9408	6.148017778	0	2.011317391	0.845861	2.857178651	-0.5528981	0.985966	6.695302
FASnCIFFI	-59.4911	6.200341333	0	1.532140784	0.624819	2.156959357	-0.5314293	0.978326	6.540497
FASnCIFF	-60.1765	6.200341333	0	2.166462771	0.905737	3.072199923	-0.5500351	1.000969 >1	6.108568
FASnCIFFCI	-59.6105	6.200341333	0	1.746549878	0.715066	2.461616264	-0.517409	0.983051	5.366914
FASnCIFFBr	-59.3412	6.200341333	0	1.465424955	0.613519	2.078943604	-0.5189426	0.978326	5.29532
FASnCIFFI	-58.9486	6.252664889	0	1.112867645	0.454445	1.567312621	-0.5022301	0.971093	5.462664
FASnBrFF	-62.8187	6.095694222	0	3.303181637	1.439046	4.742228051	-0.7396771	1.03168 >1	14.74213
FASnBrFFCI	-62.2598	6.095694222	0	2.851376182	1.176332	4.027708605	-0.7076368	1.009959 >1	15.07645 >15%
FASnBrFFBr	-62.0239	6.095694222	0	2.557725401	1.042972	3.600697162	-0.7119558	1.004277 >1	20.26157 >15%
FASnBrFI	-61.3042	6.095694222	0	1.792857377	0.700705	2.493562841	-0.6679875	0.995617	11.74618
FASnBrCIF	-60.9432	6.095694222	0	2.82244515	1.254083	4.076528123	-0.5979187	1.009959 >1	7.354317
FASnBrCICI	-60.2413	6.148017778	0	2.431471649	1.038176	3.469648078	-0.5539689	0.990963	8.5824
FASnBrCIBr	-59.9543	6.148017778	0	2.079734755	0.873738	2.953472592	-0.5540217	0.985966	8.585714
FASnBrCII	-59.4993	6.200341333	0	1.616929665	0.660381	2.277310299	-0.5321147	0.978326	8.523699
FASnBrBrF	-60.4277	6.095694222	0	2.390092815	0.999152	3.389244914	-0.5789424	1.004277 >1	5.004539
FASnBrBrCl	-59.7476	6.148017778	0	2.126086322	0.913912	3.039998097	-0.5367972	0.985966	6.198079
FASnBrBrBr	-59.4249	6.200341333	0	1.834965866	0.782608	2.617574161	-0.5338807	0.981141	6.082687
FASnBrBrI	-59.0359	6.200341333	0	1.354666739	0.556857	1.911523482	-0.5174704	0.97376	5.972849
FASnBrIF	-59.6786	6.200341333	0	1.925643057	0.809081	2.734723884	-0.5325186	0.995617	4.926018
FASnBrICI	-59.1414	6.200341333	0	1.554606943	0.641506	2.196113026	-0.5022859	0.978326	5.122774
FASnBrIBr	-58.8538	6.252664889	0	1.403950199	0.604271	2.008221697	-0.5022947	0.97376	4.857627
FASnBrII	-58.5052	6.252664889	0	0.993725097	0.410131	1.403855754	-0.48925	0.966766	5.319455
FASnIFF	-62.3316	6.095694222	0	2.228380425	0.926666	3.155046215	-0.7150899	1.021376 >1	14.51015
FASnIFCI	-61.7392	6.095694222	0	1.93382557	0.806543	2.740368407	-0.680263	1.000969 >1	14.81894
FASnIFBr	-61.2979	6.095694222	0	1.664661292	0.682084	2.346744891	-0.6674633	0.995617	12.12658
FASnIFI	-60.8587	6.200341333	0	1.605889931	0.652393	2.258283281	-0.6468678	0.987446	19.36131 >15%
FASnICIF	-60.2456	6.148017778	0	1.946220172	0.821478	2.767698215	-0.5557909	1.000969 >1	8.124101
FASnICICI	-59.6342	6.200341333	0	1.680067128	0.723086	2.403153033	-0.5193786	0.983051	7.818692
FASnICIBr	-59.3696	6.200341333	0	1.450725791	0.619241	2.069967062	-0.5213017	0.978326	8.142846
FASnICII	-58.9448	6.252664889	0	1.076531491	0.448155	1.52468626	-0.5019096	0.971093	5.916082
FASnIBrF	-59.6846	6.200341333	0	1.877730466	0.830904	2.708634141	-0.5330169	0.995617	5.985121
FASnIBrCl	-59.1509	6.200341333	0	1.483853993	0.646949	2.130802497	-0.5030804	0.978326	5.304787
FASnIBrBr	-58.85	6.252664889	0	1.347105996	0.585806	1.932912363	-0.5019838	0.97376	5.024615
FASnIBrI	-58.4951	6.252664889	0	0.991526107	0.417547	1.409073273	-0.4884074	0.966766	4.817196
FASnIIF	-59.0877	6.252664889	0	1.407621515	0.601323	2.008944542	-0.499279	0.987446	4.768948
FASnIICI	-58.587	6.252664889	0	1.152155388	0.486957	1.639112873	-0.4720915	0.971093	4.990533
FASnIIBr	-58.3512	6.252664889	0	0.910849889	0.407744	1.318593716	-0.476415	0.966766	4.877112
FASnIII	-57.9966	6.304988444	0	0.710628399	0.302548	1.013176752	-0.46287	0.960129	4.790317

Table S2 All data of Sn-Based Compositions.

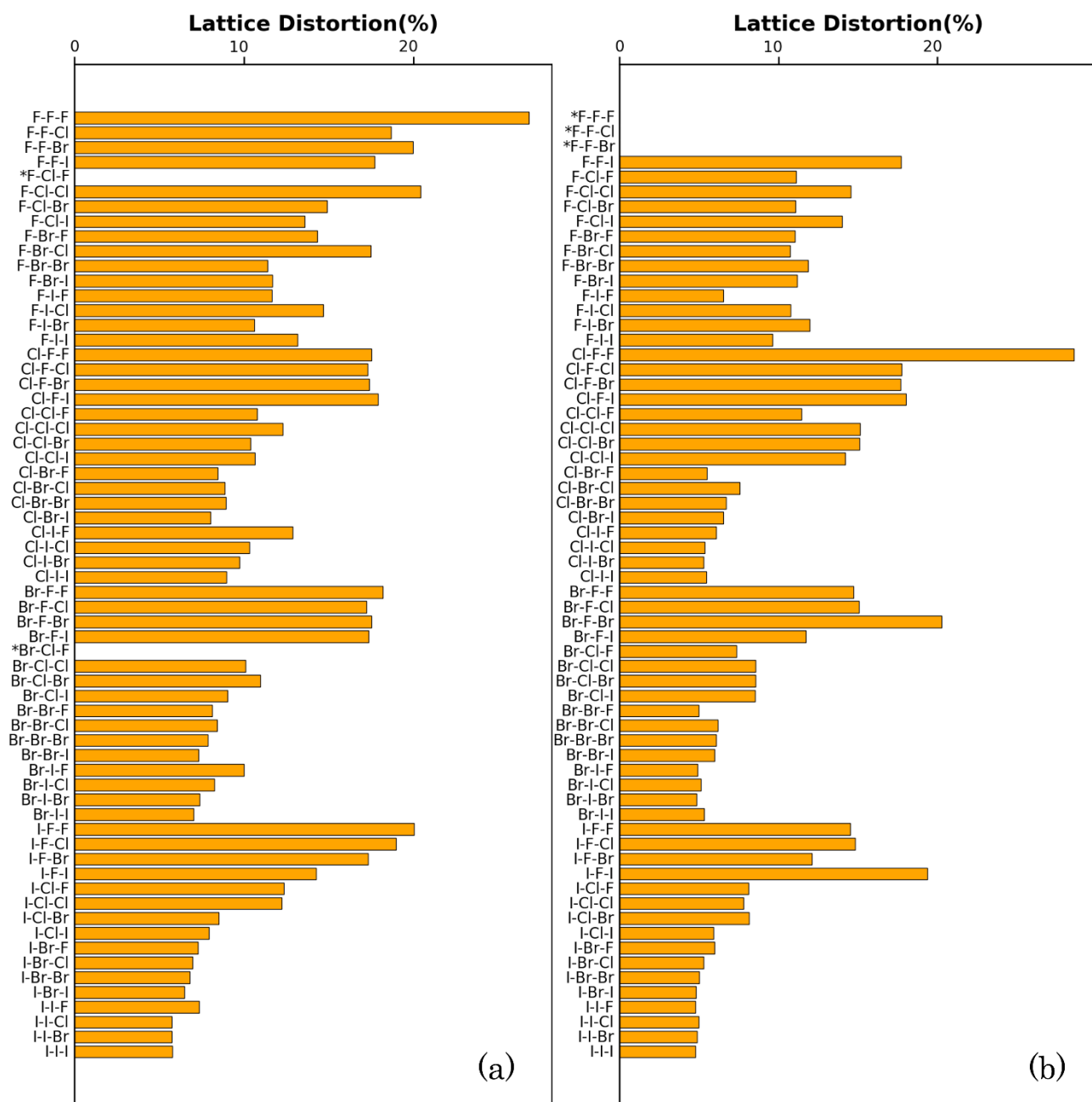


Figure S3 (a)Lattice distortion of Ge-Based Compositions (b)Lattice distortion of Sn-Based Compositions. Composition with * has no data due to convergence errors.