Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

N2O

composition	oxidation state	t	tau	Spacegroup 123						Prototypes	
				E_total (eV)	E_form (eV/atom)	E_hull (meV/atom)	structure	E_hull (meV/atom)	Gap (eV)	Magnetization	
BaNbN2O				-7.964	-1.53	247	ce00563	212	0.00	0.17	
BaReN2O	2:6:-3:-2	0.99	3.49	-8.097	-1.19	125	ce01666	-11	0.00	0.00	
BaTaN2O				-8.496	-1.71	207	ce00563	178	0.00	0.13	
BaTcN2O				-7.539	-1.05	205	ce01666	79	0.00	0.00	
CaReN2O	2:6:-3:-2	0.87	4.47	-8.158	-1.24	146	ce00563	-5	0.00	0.00	
KReN2O	1:7:-3:-2	1.01	3.71	-7.462	-0.72	248	icsd84635a	7	1.94	0.00	
LaNbN2O	3:5:-3:-2	0.84	3.74	-8.991	-1.95	127	ce00563	-32	1.12	0.00	
LaReN2O	3:5:-3:-2	0.87	2.83	-9.036	-1.53	128	ce00563	22	0.00	0.00	
LaTaN2O	3:5:-3:-2	0.84	3.74	-9.545	-2.16	80	ce00563	-45	1.29	0.00	
LaTcN2O	3:5:-3:-2	0.86	3.09	-8.539	-1.45	170	ce00563	47	0.00	0.00	
NaReN2O	1:7:-3:-2	0.88	4.09	-7.526	-0.74	213	icsd84635a	46	1.89	0.00	
PbReN2O	2:6:-3:-2	0.93	3.76	-7.702	-0.44	208	ce01666	70	0.00	0.00	
SrNbN2O				-7.955	-1.57	242	ce00563	209	0.00	0.10	
SrReN2O	2:6:-3:-2	0.93	3.78	-8.137	-1.28	81	ce01666	-53	0.00	0.00	
SrTaN2O				-8.506	-1.77	201	icsd68098a	52	1.99	0.00	
SrTcN2O				-7.561	-1.12	208	ce01666	78	0.00	0.00	

composition	oxidation state	t	tau	Spacegroup 123			Prototypes			
				E_total (eV)	E_form (eV/atom)	E_hull (meV/atom)	structure	E_hull (meV/atom)	Gap (eV)	Magnetization
BaMoO2N	2:5:-2:-3	0.96	3.49	-6.981	-1.85	201	ce00563	124	0.76	0.20
BaNbO2N	2:5:-2:-3	0.95	3.54	-8.152	-2.46	65	ce00563	-22	1.25	0.00
BaOsO2N	2:5:-2:-3	0.98	3.47	-7.415	-1.50	210	ce01666	98	0.00	0.00
BaReO2N	2:5:-2:-3	0.98	3.47	-7.993	-1.83	94	ce01666	-41	0.00	0.00
BaRuO2N	2:5:-2:-3	0.99	3.46	-6.984	-1.46	240	ce01666	130	0.00	0.00
BaTaO2N	2:5:-2:-3	0.95	3.54	-8.688	-2.64	33	ce00112	-44	1.43	0.00
BaTcO2N	2:5:-2:-3	0.97	3.48	-7.516	-1.77	82	ce01666	-54	0.00	0.00
CaNbO2N	2:5:-2:-3	0.83	5.34	-8.115	-2.41	193	ce00563	22	1.81	0.00
CaReO2N	2:5:-2:-3	0.86	4.67	-8.009	-1.83	164	ce00112	-5	0.41	0.00
CaTaO2N	2:5:-2:-3	0.83	5.34	-8.688	-2.63	146	ce00563	13	1.67	0.00
CaTcO2N	2:5:-2:-3	0.85	4.86	-7.519	-1.76	176	ce00112	-7	0.44	0.00
KReO2N	1:6:-2:-3	1.01	3.64	-7.446	-1.45	124	ce00112	25	0.00	0.00
KTcO2N				-6.847	-1.27	223	icsd84635a	115	0.51	0.20
LaHfO2N	3:4:-2:-3	0.81	5.38	-9.320	-3.05	177	ce00563	20	2.53	0.00
LaNbO2N	3:4:-2:-3	0.83	4.57	-8.887	-2.59	258	ce00112	143	0.00	0.00
LaTaO2N	3:4:-2:-3	0.83	4.57	-9.372	-2.72	220	ce00112	140	0.00	0.00
LaTcO2N	3:4:-2:-3	0.84	3.81	-8.386	-2.04	243	ce00563	76	0.00	0.01
LaTiO2N	3:4:-2:-3	0.86	3.13	-8.822	-2.97	121	ce00563	30	1.64	0.00
LaZrO2N	3:4:-2:-3	0.81	5.70	-8.852	-2.87	260	ce00563	45	2.53	0.00
LiReO2N	1:6:-2:-3	0.78	5.76	-7.561	-1.40	223	ce00563	40	0.00	0.00
NaOsO2N	1:6:-2:-3	0.88	4.08	-6.802	-1.01	228	ce01666	83	0.00	0.00
NaReO2N	1:6:-2:-3	0.88	4.09	-7.497	-1.46	92	ce00112	-7	0.00	0.00
NaTcO2N				-6.890	-1.27	175	ce00112	79	0.00	0.00
PbReO2N	2:5:-2:-3	0.92	3.80	-7.562	-1.04	171	ce01666	34	0.00	0.00
PbTaO2N	2:5:-2:-3	0.90	4.03	-8.290	-1.89	152	ce00563	86	1.95	0.00
PbTcO2N	2:5:-2:-3	0.91	3.86	-7.088	-0.98	211	ce01666	62	0.00	0.00
RbReO2N	1:6:-2:-3	1.06	3.60	-7.299	-1.33	246	ce00112	147	0.00	0.00
SnTaO2N				-8.260	-1.80	247	icsd68098a	126	2.30	0.00
SrMoO2N	2:5:-2:-3	0.91	3.93	-6.965	-1.88	240	ce00563	148	0.65	0.20
SrNbO2N	2:5:-2:-3	0.89	4.07	-8.135	-2.49	72	ce00563	-21	1.37	0.00
SrOsO2N	2:5:-2:-3	0.92	3.81	-7.419	-1.55	202	ce01666	94	0.00	0.00
SrReO2N	2:5:-2:-3	0.92	3.83	-8.009	-1.89	87	ce01666	-47	0.00	0.00
SrRuO2N	2:5:-2:-3	0.93	3.79	-6.978	-1.50	251	ce01666	134	0.00	0.00

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SrTaO2N	2:5:-2:-3	0.89	4.07	-8.693	-2.70	65	ce00112	-14	1.68	0.00
SrTcO2N	2:5:-2:-3	0.91	3.89	-7.523	-1.82	95	ce01666	-47	0.00	0.00

composition	oxidation state	t	tau	Spacegroup 123			Prototypes			
				E_total (eV)	E_form (eV/atom)	E_hull (meV/atom)	structure	E_hull (meV/atom)	Gap (eV)	Magnetization
AgAlF2O	1:3:-1:-2	0.94	3.75	-5.262	-2.53	229	icsd84635a	100	1.88	0.00
AgCoF2O	1:3:-1:-2	0.90	3.79	-4.472	-1.44	209	icsd84635a	186	0.57	0.80
AgCuF2O	1:3:-1:-2	0.93	3.75	-3.906	-1.11	176	icsd84635a	33	0.00	0.00
AgFeF2O	1:3:-1:-2	0.89	3.85	-4.877	-1.75	152	icsd68098a	64	1.18	1.00
AgGaF2O	1:3:-1:-2	0.90	3.80	-4.493	-1.91	161	icsd84635a	42	1.16	0.00
AgInF2O	1:3:-1:-2	0.82	4.63	-4.296	-1.76	201	icsd84635a	77	0.40	0.00
AgPdF2O	2:2:-1:-2	0.73	25.28	-3.991	-0.97	222	ce00563	63	0.00	0.02
AgScF2O	1:3:-1:-2	0.84	4.24	-6.109	-2.86	213	ce00563	111	1.68	0.00
AgTlF2O	1:3:-1:-2	0.79	5.66	-3.691	-1.24	249	icsd84635a	57	0.01	0.00
BaCaF2O	2:2:-1:-2	0.81	6.83	-5.809	-3.61	226	ce00563	123	3.42	0.00
BaFeF2O	2:2:-1:-2	0.90	4.04	-5.945	-3.00	204	ce00112	179	2.90	0.80
BaLiF2O				-5.145	-2.96	247	ce01402	34	3.38	0.00
BaMgF2O	2:2:-1:-2	0.92	3.72	-5.692	-3.57	162	ce01666	130	3.92	0.00
BaMnF2O	2:2:-1:-2	0.88	4.41	-6.373	-3.08	232	ce00112	173	2.06	1.00
BaNiF2O				-5.149	-2.62	300	ce01666	259	2.83	0.40
CsAgF2O	1:3:-1:-2	1.02	3.23	-3.759	-1.60	191	icsd68098a	115	1.10	0.01
CsAuF2O	1:3:-1:-2	0.97	3.26	-3.771	-1.52	231	ce00563	82	0.36	0.00
CsBiF2O	1:3:-1:-2	0.90	3.58	-4.740	-2.37	120	ce00112	3	2.60	0.00
CsCaF2O				-4.946	-2.95	218	icsd68098a	40	3.01	0.01
CsCoF2O	1:3:-1:-2	1.09	3.36	-4.709	-2.07	179	ce00112	69	1.13	0.81
CsCuF2O	1:3:-1:-2	1.13	3.50	-4.166	-1.75	232	icsd68098a	72	1.41	0.00
CsFeF2O	1:3:-1:-2	1.07	3.31	-5.094	-2.35	263	ce00112	115	2.69	1.00
CsHgF2O				-3.334	-1.68	176	icsd68098a	-20	0.55	0.20
CsInF2O	1:3:-1:-2	0.99	3.23	-4.630	-2.48	172	icsd68098a	83	2.48	0.00
CsLaF2O	1:3:-1:-2	0.90	3.59	-6.164	-3.58	125	ce00112	79	4.19	0.01
CsMnF2O	1:3:-1:-2	1.07	3.31	-5.527	-2.43	204	icsd68098a	53	0.61	0.80
CsMoF2O	1:3:-1:-2	1.05	3.26	-5.433	-2.37	175	icsd68098a	99	1.82	0.60
CsPbF2O				-4.641	-2.30	64	ce01402	50	1.12	0.00
CsPdF2O				-4.359	-1.73	223	ce01402	156	0.00	0.12
CsSbF2O	1:3:-1:-2	1.01	3.23	-4.727	-2.31	230	ce00112	30	3.83	0.00
CsScF2O	1:3:-1:-2	1.02	3.23	-6.354	-3.49	206	ce00112	136	4.23	0.00
CsSnF2O				-4.819	-2.43	186	ce01402	90	1.76	0.00
CsSrF2O				-4.819	-2.88	242	ce01402	44	2.83	0.00

CsTiF2O	1:3:-1:-2	1.06	3.28	-6.253	-3.08	223	ce00112	143	0.41	0.20
CsTlF2O	1:3:-1:-2	0.96	3.29	-4.129	-2.06	109	ce01402	108	0.33	0.00
CsVF2O	1:3:-1:-2	1.07	3.31	-5.776	-2.70	213	ce00112	178	1.80	0.40
CsYF2O	1:3:-1:-2	0.95	3.31	-6.456	-3.57	149	ce00112	86	4.69	0.00
HgCuF2O	2:2:-1:-2	0.81	6.66	-3.446	-1.15	268	ce00563	65	0.11	0.00
InGaF2O				-4.659	-2.09	237	ce00112	72	2.67	0.00
InMoF2O				-5.392	-1.96	241	ce00563	168	1.31	0.60
KAgF2O	1:3:-1:-2	0.92	3.55	-3.803	-1.60	198	icsd68098a	13	0.75	0.20
KAlF2O	1:3:-1:-2	1.02	3.57	-5.608	-3.22	218	icsd84635a	43	4.51	0.00
KAsF2O	1:3:-1:-2	1.00	3.51	-4.738	-2.17	255	icsd68098a	24	4.32	0.00
KBiF2O	1:3:-1:-2	0.81	5.00	-4.761	-2.35	181	icsd84635a	-2	3.18	0.00
KCoF2O	1:3:-1:-2	0.98	3.49	-4.891	-2.21	87	ce00563	71	0.61	0.00
KCrF2O				-5.777	-2.61	262	ce00112	195	1.26	0.60
KCuF2O	1:3:-1:-2	1.02	3.56	-4.307	-1.85	168	icsd68098a	106	0.42	0.20
KFeF2O	1:3:-1:-2	0.97	3.48	-5.278	-2.49	132	ce00112	106	1.75	1.00
KGaF2O	1:3:-1:-2	0.98	3.48	-4.888	-2.64	174	ce00563	98	3.53	0.01
KGeF2O				-4.928	-2.37	236	ce00563	73	3.27	0.00
KHgF2O				-3.359	-1.66	200	icsd84635a	165	0.00	0.00
KLaF2O	1:3:-1:-2	0.81	5.02	-6.162	-3.54	208	icsd84635a	65	4.12	0.00
KMgF2O				-4.739	-2.78	243	icsd68098a	79	3.06	0.01
KMnF2O	1:3:-1:-2	0.97	3.48	-5.696	-2.57	109	ce00112	87	0.51	0.80
KMoF2O	1:3:-1:-2	0.95	3.49	-5.544	-2.44	198	ce00112	135	2.20	0.60
KNiF2O	1:3:-1:-2	0.99	3.49	-4.246	-1.88	195	ce00002	195	0.00	0.58
KPbF2O				-4.660	-2.28	110	ce01402	91	0.85	0.00
KPdF2O				-4.455	-1.78	177	icsd84635a	111	0.00	0.00
KRhF2O	1:3:-1:-2	0.96	3.48	-5.023	-1.92	205	ce00563	176	0.32	0.10
KRuF2O	1:3:-1:-2	0.95	3.48	-5.467	-1.97	235	icsd84635a	179	0.00	0.05
KSbF2O	1:3:-1:-2	0.91	3.57	-4.771	-2.31	245	ce00112	21	4.19	0.00
KScF2O	1:3:-1:-2	0.92	3.55	-6.498	-3.59	125	ce00112	58	4.62	0.00
KSnF2O				-4.877	-2.44	195	ce00563	103	2.04	0.00
KTiF2O	1:3:-1:-2	0.96	3.48	-6.426	-3.21	124	ce01666	71	0.00	0.20
KTlF2O	1:3:-1:-2	0.86	3.95	-4.169	-2.06	139	icsd68098a	91	1.36	0.00
KVF2O	1:3:-1:-2	0.97	3.48	-5.957	-2.84	124	ce00112	74	1.92	0.40
KYF2O	1:3:-1:-2	0.86	4.02	-6.512	-3.58	155	icsd84635a	59	4.14	0.00
KZnF2O				-4.047	-2.16	244	ce00563	131	0.11	0.10

LaLiF2O	3:1:-1:-2	0.80	7.14	-6.373	-3.59	248	icsd68098a	104	4.99	0.00
NaAlF2O	1:3:-1:-2	0.89	3.97	-5.660	-3.23	190	icsd84635a	26	4.84	0.00
NaCoF2O	1:3:-1:-2	0.85	4.16	-4.856	-2.13	146	ce00563	98	0.64	0.40
NaCuF2O	1:3:-1:-2	0.89	3.98	-4.293	-1.79	203	icsd68098a	108	0.61	0.01
NaFeF2O	1:3:-1:-2	0.84	4.33	-5.241	-2.41	165	icsd84635a	44	2.31	1.00
NaGaF2O	1:3:-1:-2	0.85	4.21	-4.871	-2.59	202	icsd84635a	25	3.65	0.00
NaInF2O	1:3:-1:-2	0.78	6.16	-4.635	-2.41	246	icsd84635a	103	2.16	0.00
NaMnF2O	1:3:-1:-2	0.84	4.33	-5.653	-2.48	162	icsd68098a	44	0.24	0.80
NaScF2O	1:3:-1:-2	0.80	5.22	-6.439	-3.49	196	icsd84635a	72	4.91	0.00
NaTiF2O	1:3:-1:-2	0.83	4.49	-6.378	-3.12	176	icsd84635a	64	0.00	0.07
NaVF2O	1:3:-1:-2	0.84	4.30	-5.915	-2.76	145	ce00112	69	1.91	0.40
PbMgF2O	2:2:-1:-2	0.87	4.50	-5.233	-2.75	146	ce00563	73	2.95	0.00
PbMnF2O	2:2:-1:-2	0.82	5.94	-5.855	-2.20	219	ce00563	59	1.43	1.00
RbAgF2O	1:3:-1:-2	0.97	3.36	-3.776	-1.60	189	icsd68098a	1	0.46	0.20
RbAsF2O	1:3:-1:-2	1.05	3.45	-4.698	-2.15	256	ce00563	22	3.55	0.00
RbAuF2O	1:3:-1:-2	0.92	3.47	-3.802	-1.54	226	ce00563	92	0.37	0.00
RbBiF2O	1:3:-1:-2	0.85	4.09	-4.752	-2.36	133	icsd84635a	-17	3.24	0.00
RbCaF2O				-4.941	-2.93	256	ce01402	56	2.92	0.01
RbCdF2O				-3.814	-2.02	237	ce00563	118	0.12	0.10
RbCoF2O	1:3:-1:-2	1.03	3.40	-4.817	-2.16	118	ce00563	115	0.78	0.80
RbCuF2O	1:3:-1:-2	1.07	3.52	-4.264	-1.83	170	icsd68098a	46	0.99	0.01
RbFeF2O	1:3:-1:-2	1.02	3.37	-5.204	-2.44	171	ce00112	151	1.72	1.00
RbGaF2O	1:3:-1:-2	1.03	3.39	-4.802	-2.58	212	ce00563	91	3.28	0.00
RbHgF2O				-3.348	-1.67	167	icsd68098a	-31	0.89	0.20
RbInF2O	1:3:-1:-2	0.94	3.40	-4.687	-2.52	147	ce00002	147	1.23	0.00
RbLaF2O	1:3:-1:-2	0.85	4.10	-6.161	-3.56	159	icsd84635a	60	3.97	0.00
RbMgF2O				-4.685	-2.75	244	ce00563	123	2.46	0.01
RbMnF2O	1:3:-1:-2	1.02	3.37	-5.627	-2.52	141	icsd68098a	94	2.18	0.80
RbMoF2O	1:3:-1:-2	0.99	3.35	-5.501	-2.42	138	ce00112	78	2.03	0.60
RbNiF2O	1:3:-1:-2	1.04	3.42	-4.177	-1.84	252	ce00002	252	0.00	0.59
RbPbF2O				-4.652	-2.30	74	ce01402	60	1.11	0.00
RbPdF2O				-4.416	-1.77	182	ce01402	136	0.00	0.12
RbRhF2O	1:3:-1:-2	1.01	3.36	-4.979	-1.90	217	ce00563	167	0.24	0.10
RbRuF2O	1:3:-1:-2	1.00	3.35	-5.418	-1.95	248	ce00563	232	0.09	0.20
RbSbF2O	1:3:-1:-2	0.96	3.36	-4.754	-2.31	209	ce00112	17	3.73	0.00

RbScF2O	1:3:-1:-2	0.97	3.35	-6.441	-3.56	143	ce00112	76	4.44	0.00
RbSnF2O				-4.854	-2.44	178	ce00563	101	1.92	0.00
RbTcF2O				-5.795	-2.11	201	icsd68098a	-24	0.03	0.00
RbTiF2O	1:3:-1:-2	1.00	3.35	-6.358	-3.17	135	ce01666	84	0.00	0.20
RbTlF2O	1:3:-1:-2	0.91	3.54	-4.153	-2.07	118	icsd84635a	107	0.97	0.00
RbVF2O	1:3:-1:-2	1.02	3.37	-5.886	-2.79	153	ce00112	111	1.91	0.40
RbYF2O	1:3:-1:-2	0.90	3.58	-6.489	-3.58	135	ce00112	70	4.31	0.01
SrMgF2O	2:2:-1:-2	0.86	4.58	-5.624	-3.55	226	ce00112	167	4.18	0.00
TlBiF2O	1:3:-1:-2	0.85	4.19	-4.634	-1.97	165	icsd84635a	21	2.87	0.00
TlCoF2O	1:3:-1:-2	1.03	3.41	-4.687	-1.75	170	icsd84635a	158	1.01	0.80
TlCuF2O	3:1:-1:-2	0.75	20.73	-4.144	-1.43	249	icsd68098a	109	0.51	0.00
TlFeF2O	1:3:-1:-2	1.01	3.38	-5.074	-2.04	164	ce00563	127	1.68	1.00
TlGaF2O	1:3:-1:-2	1.02	3.40	-4.660	-2.17	214	icsd84635a	40	3.24	0.00
TlInF2O	1:3:-1:-2	0.94	3.43	-4.568	-2.13	118	icsd84635a	95	1.95	0.00
TlLaF2O	1:3:-1:-2	0.85	4.20	-6.052	-3.18	181	icsd68098a	52	2.96	0.00
TlMgF2O				-4.722	-2.51	203	ce00563	123	1.26	0.00
TlMnF2O	1:3:-1:-2	1.01	3.38	-5.507	-2.12	148	icsd68098a	66	0.61	0.80
TlMoF2O	1:3:-1:-2	0.99	3.36	-5.398	-2.05	153	icsd68098a	70	0.00	0.60
TlNiF2O	1:3:-1:-2	1.03	3.42	-4.127	-1.51	262	ce00563	147	0.35	0.40
TlPbF2O				-4.517	-1.88	156	ce01402	134	1.27	0.00
TlPdF2O				-4.288	-1.36	259	ce00563	191	0.00	0.05
TlRhF2O	1:3:-1:-2	1.00	3.37	-4.846	-1.49	195	ce00563	109	0.00	0.07
TlRuF2O	1:3:-1:-2	0.99	3.37	-5.290	-1.55	254	ce01402	197	0.00	0.01
TlSbF2O	1:3:-1:-2	0.95	3.38	-4.632	-1.92	222	icsd68098a	18	3.08	0.00
TlScF2O	1:3:-1:-2	0.96	3.38	-6.327	-3.17	119	ce00112	56	3.60	0.00
TlSnF2O				-4.724	-2.04	191	ce01402	81	2.17	0.00
TlTcF2O				-5.663	-1.70	246	icsd84635a	171	0.00	0.00
TlTiF2O	1:3:-1:-2	1.00	3.37	-6.229	-2.76	201	icsd84635a	128	0.00	0.06
TlVF2O	1:3:-1:-2	1.01	3.38	-5.755	-2.38	134	ce01402	100	1.27	0.40
TlYF2O	1:3:-1:-2	0.90	3.63	-6.393	-3.21	137	icsd84635a	50	2.39	0.00
TlZnF2O				-3.940	-1.80	247	ce00563	123	0.99	0.00

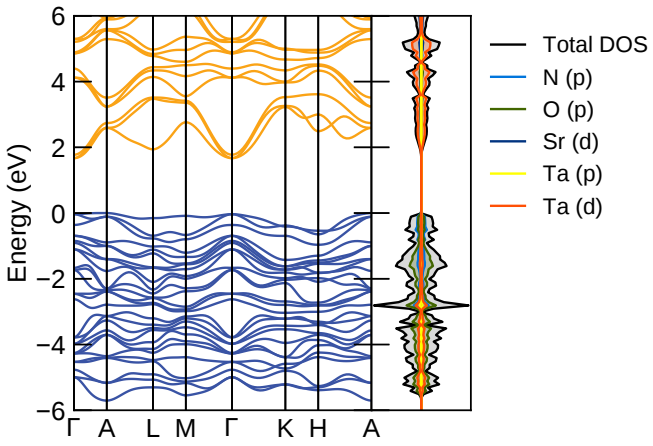
composition	oxidation state	t	tau	Spacegroup 123			Prototypes			
				E_total (eV)	E_form (eV/atom)	E_hull (meV/atom)	structure	E_hull (meV/atom)	Gap (eV)	Magnetization
AgAlO2F	2:3:-2:-1	0.86	4.64	-5.408	-2.11	276	ce00563	221	0.00	0.08
AgFeO2F	2:3:-2:-1	0.81	6.20	-4.982	-1.29	269	icsd68098a	117	0.00	0.82
AgHfO2F	1:4:-2:-1	0.86	4.09	-7.308	-2.77	183	ce00112	64	1.76	0.00
AgOsO2F	1:4:-2:-1	0.89	3.85	-5.868	-1.07	242	ce00563	131	0.00	0.00
AgSnO2F	1:4:-2:-1	0.86	4.01	-4.892	-1.55	228	icsd68098a	76	0.15	0.00
AgTcO2F	1:4:-2:-1	0.88	3.88	-6.020	-1.40	250	ce00563	187	0.41	0.00
AgTiO2F	1:4:-2:-1	0.90	3.81	-6.595	-2.47	141	icsd84635a	26	2.17	0.00
AgZrO2F	1:4:-2:-1	0.85	4.14	-6.880	-2.62	204	ce00563	69	1.97	0.00
BaAgO2F	2:3:-2:-1	0.91	3.89	-4.819	-1.89	233	icsd84635a	140	0.00	0.03
BaCoO2F	2:3:-2:-1	0.97	3.44	-5.819	-2.41	185	ce00112	133	0.52	0.80
BaCrO2F				-6.757	-2.86	223	ce00112	152	1.39	0.60
BaCuO2F	2:3:-2:-1	1.01	3.41	-5.354	-2.17	189	icsd84635a	146	0.00	0.02
BaFeO2F	2:3:-2:-1	0.95	3.50	-6.202	-2.69	130	ce00112	56	1.52	1.00
BaGaO2F	2:3:-2:-1	0.97	3.45	-5.814	-2.84	248	icsd68098a	110	3.52	0.00
BaInO2F	2:3:-2:-1	0.89	4.20	-5.621	-2.71	146	ce00112	82	2.05	0.00
BaMgO2F				-5.668	-2.98	180	ce00002	180	0.00	0.20
BaMnO2F	2:3:-2:-1	0.95	3.50	-6.671	-2.81	92	ce00112	64	0.00	0.80
BaMoO2F	2:3:-2:-1	0.93	3.63	-6.501	-2.67	223	ce00112	155	2.23	0.60
BaNiO2F	2:3:-2:-1	0.98	3.43	-5.229	-2.14	212	ce00563	207	0.00	0.20
BaScO2F	2:3:-2:-1	0.91	3.86	-7.385	-3.75	90	ce00112	13	4.11	0.00
BaTiO2F	2:3:-2:-1	0.94	3.56	-7.357	-3.41	177	ce00112	105	0.00	0.20
BaTlO2F	2:3:-2:-1	0.85	4.98	-5.045	-2.21	222	icsd84635a	75	1.98	0.00
BaVO2F	2:3:-2:-1	0.96	3.49	-6.899	-3.05	87	ce00112	57	0.80	0.40
BaYO2F	2:3:-2:-1	0.85	5.16	-7.316	-3.66	164	ce00563	56	4.09	0.00
BaZnO2F				-5.072	-2.45	202	ce01402	201	0.00	0.10
CaAlO2F	2:3:-2:-1	0.88	4.28	-6.624	-3.49	211	icsd84635a	130	3.82	0.00
CdAlO2F	2:3:-2:-1	0.86	4.57	-5.451	-2.54	224	icsd84635a	58	2.20	0.00
CsBiO2F				-4.861	-1.92	107	ce01666	73	0.00	0.00
CsLaO2F				-6.096	-2.95	236	icsd68098a	144	3.20	0.00
CsNbO2F	1:4:-2:-1	1.05	3.30	-6.844	-2.66	242	icsd84635a	97	0.00	0.03
CsPbO2F	1:4:-2:-1	1.00	3.25	-4.661	-1.76	171	icsd84635a	103	1.18	0.01
CsSbO2F				-5.003	-2.02	248	ce01402	119	0.00	0.00
CsTeO2F	1:4:-2:-1	0.92	3.45	-4.619	-1.83	254	ce00563	40	2.41	0.00

CsZrO2F	1:4:-2:-1	1.03	3.27	-7.085	-3.21	223	icsd68098a	108	3.91	0.00
HgAlO2F	2:3:-2:-1	0.89	4.18	-4.972	-2.18	275	icsd68098a	67	2.15	0.00
InHfO2F				-7.479	-2.96	248	icsd68098a	130	1.61	0.00
InZrO2F				-7.081	-2.84	231	icsd84635a	134	1.41	0.00
KAlO2F				-5.645	-2.69	276	ce00563	166	0.34	0.10
KBiO2F				-4.942	-1.96	112	ce00563	75	0.21	0.00
KCoO2F	1:4:-2:-1	1.02	3.62	-4.943	-1.69	190	icsd84635a	146	0.37	0.60
KFeO2F				-5.323	-1.97	171	icsd68098a	150	0.93	0.80
KGaO2F				-4.887	-2.08	255	ce00563	14	1.06	0.10
KHfO2F	1:4:-2:-1	0.93	3.53	-7.655	-3.46	141	ce00112	36	4.40	0.00
KInO2F				-4.694	-1.94	257	icsd84635a	187	1.18	0.00
KMnO2F	1:4:-2:-1	1.02	3.62	-5.749	-2.05	237	icsd68098a	150	0.96	0.60
KMoO2F	1:4:-2:-1	0.96	3.51	-5.973	-2.31	156	ce00563	117	0.93	0.40
KNbO2F	1:4:-2:-1	0.95	3.51	-7.036	-2.81	124	ce01666	28	0.00	0.00
KOsO2F	1:4:-2:-1	0.97	3.51	-6.252	-1.80	189	ce01402	104	0.00	0.03
KPbO2F	1:4:-2:-1	0.91	3.62	-4.751	-1.80	162	icsd68098a	99	1.19	0.01
KRuO2F	1:4:-2:-1	0.98	3.51	-5.867	-1.81	253	ce01402	172	0.00	0.00
KSbO2F				-5.144	-2.11	192	ce00563	117	0.17	0.00
KScO2F				-6.472	-3.00	204	ce01666	200	0.00	0.20
KSnO2F	1:4:-2:-1	0.94	3.52	-5.259	-2.26	198	icsd68098a	100	2.52	0.00
KTaO2F	1:4:-2:-1	0.95	3.51	-7.444	-2.87	229	ce01666	129	0.00	0.00
KTcO2F	1:4:-2:-1	0.96	3.51	-6.399	-2.12	194	ce01666	152	0.00	0.00
KTeO2F	1:4:-2:-1	0.83	4.47	-4.722	-1.89	216	icsd68098a	42	3.01	0.00
KTiO2F	1:4:-2:-1	0.98	3.52	-6.942	-3.16	148	icsd84635a	11	3.61	0.00
KWO2F	1:4:-2:-1	0.96	3.51	-6.143	-2.22	165	ce00112	144	1.65	0.40
KZrO2F	1:4:-2:-1	0.93	3.54	-7.248	-3.34	140	ce00112	38	3.78	0.00
NaAlO2F				-5.718	-2.72	247	ce00563	206	3.17	0.00
NaBiO2F				-4.845	-1.82	243	ce00563	96	0.42	0.00
NaCoO2F	1:4:-2:-1	0.89	4.00	-4.961	-1.67	229	icsd84635a	186	0.24	0.60
NaFeO2F				-5.332	-1.94	218	icsd68098a	206	1.01	0.80
NaHfO2F	1:4:-2:-1	0.81	4.84	-7.621	-3.39	219	ce00563	93	4.26	0.00
NaMoO2F	1:4:-2:-1	0.84	4.39	-5.933	-2.22	240	ce00563	144	1.18	0.40
NaNbO2F	1:4:-2:-1	0.82	4.59	-6.991	-2.73	207	ce00563	108	0.00	0.04
NaTiO2F	1:4:-2:-1	0.86	4.18	-6.956	-3.13	158	icsd84635a	31	3.52	0.00
NaVO2F	1:4:-2:-1	0.87	4.10	-6.250	-2.52	149	icsd84635a	-2	2.40	0.20

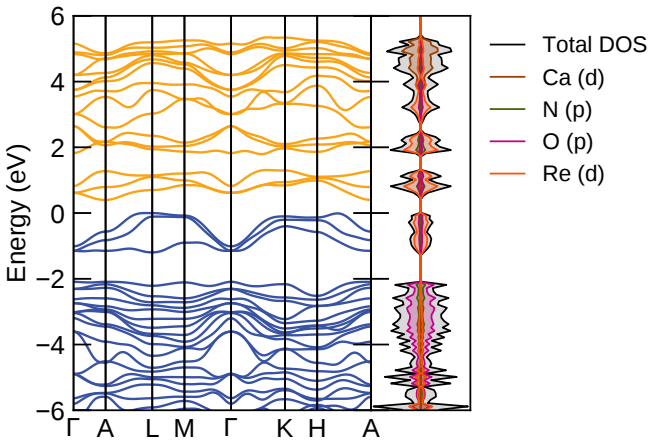
NaZrO2F	1:4:-2:-1	0.81	4.95	-7.195	-3.24	237	ce00563	99	3.97	0.00
PbAlO2F	2:3:-2:-1	0.95	3.64	-6.107	-2.63	209	icsd84635a	56	2.94	0.00
PbCoO2F	2:3:-2:-1	0.91	3.84	-5.340	-1.57	226	icsd84635a	132	0.88	0.80
PbFeO2F	2:3:-2:-1	0.90	4.00	-5.742	-1.87	195	icsd84635a	81	2.04	1.00
PbGaO2F	2:3:-2:-1	0.91	3.88	-5.353	-2.02	243	icsd84635a	70	2.89	0.00
PbMnO2F	2:3:-2:-1	0.90	4.00	-6.191	-1.97	155	icsd84635a	70	0.52	0.80
PbScO2F	2:3:-2:-1	0.86	4.78	-6.917	-2.93	173	icsd84635a	54	2.82	0.00
RbBiO2F				-4.911	-1.96	83	ce01666	50	0.00	0.00
RbCoO2F	1:4:-2:-1	1.07	3.58	-4.835	-1.61	248	icsd84635a	146	0.37	0.60
RbFeO2F				-5.219	-1.89	231	icsd84635a	175	0.00	0.80
RbHfO2F	1:4:-2:-1	0.98	3.37	-7.578	-3.41	169	ce00112	63	4.27	0.00
RbInO2F				-4.647	-1.92	241	icsd84635a	181	1.14	0.00
RbIO2F				-3.904	-1.42	231	ce00563	15	2.07	0.00
RbLaO2F				-6.108	-2.94	253	ce00002	253	0.00	0.20
RbMoO2F	1:4:-2:-1	1.01	3.40	-5.899	-2.26	180	ce01666	141	0.25	0.40
RbNbO2F	1:4:-2:-1	1.00	3.38	-6.963	-2.76	144	ce01666	44	0.00	0.00
RbOsO2F	1:4:-2:-1	1.02	3.41	-6.192	-1.77	199	ce01402	138	0.00	0.02
RbPbO2F	1:4:-2:-1	0.95	3.40	-4.715	-1.80	147	icsd68098a	114	0.15	0.00
RbSbO2F				-5.090	-2.09	189	ce00563	98	1.28	0.00
RbScO2F				-6.410	-2.97	223	ce01402	221	0.05	0.20
RbSnO2F	1:4:-2:-1	0.99	3.38	-5.184	-2.21	223	icsd84635a	189	1.71	0.01
RbTaO2F	1:4:-2:-1	1.00	3.38	-7.362	-2.81	249	ce01666	144	0.00	0.00
RbTcO2F	1:4:-2:-1	1.01	3.40	-6.316	-2.07	226	ce01402	144	0.00	0.01
RbTeO2F	1:4:-2:-1	0.87	3.83	-4.683	-1.88	182	ce00563	10	2.38	0.00
RbTiO2F	1:4:-2:-1	1.03	3.44	-6.829	-3.07	205	icsd84635a	2	3.59	0.00
RbTlO2F				-4.109	-1.46	253	ce00563	132	0.00	0.01
RbVO2F	1:4:-2:-1	1.05	3.48	-6.120	-2.46	229	icsd84635a	16	2.40	0.20
RbWO2F	1:4:-2:-1	1.01	3.39	-6.069	-2.17	197	ce00112	178	1.60	0.40
RbYO2F				-6.440	-2.97	240	ce01666	237	0.00	0.20
RbZrO2F	1:4:-2:-1	0.98	3.37	-7.186	-3.30	152	ce00112	51	3.66	0.00
SrAlO2F	2:3:-2:-1	0.95	3.66	-6.570	-3.50	202	ce00112	126	4.81	0.00
SrCoO2F	2:3:-2:-1	0.91	3.88	-5.794	-2.43	180	icsd84635a	110	1.41	0.80
SrCrO2F				-6.747	-2.90	253	ce00112	179	1.81	0.60
SrCuO2F	2:3:-2:-1	0.94	3.67	-5.326	-2.19	178	icsd68098a	42	0.84	0.00
SrFeO2F	2:3:-2:-1	0.89	4.05	-6.169	-2.70	171	ce00112	90	1.57	1.00

SrGaO2F	2:3:-2:-1	0.91	3.92	-5.806	-2.88	249	ce00112	169	2.60	0.00
SrMgO2F				-5.602	-2.96	243	ce00563	186	0.00	0.10
SrMnO2F	2:3:-2:-1	0.89	4.05	-6.629	-2.81	139	icsd68098a	88	2.05	0.80
SrNiO2F	2:3:-2:-1	0.91	3.84	-5.206	-2.16	233	ce00563	215	0.00	0.20
SrScO2F	2:3:-2:-1	0.85	4.86	-7.312	-3.73	172	ce00563	62	4.18	0.00
SrTiO2F	2:3:-2:-1	0.88	4.20	-7.311	-3.41	227	ce00112	151	0.00	0.20
SrVO2F	2:3:-2:-1	0.90	4.02	-6.860	-3.06	109	ce00563	62	1.24	0.40
SrZnO2F				-5.019	-2.45	253	icsd84635a	216	0.00	0.00
TlBiO2F				-4.798	-1.57	192	icsd84635a	121	0.00	0.00
TlHfO2F	1:4:-2:-1	0.97	3.39	-7.480	-3.03	179	ce00112	80	3.56	0.00
TlIO2F				-3.776	-1.02	241	ce00563	15	2.00	0.00
TlIrO2F	1:4:-2:-1	1.02	3.43	-5.511	-1.29	267	ce01402	224	0.00	0.04
TlMoO2F	1:4:-2:-1	1.00	3.41	-5.788	-1.87	204	ce01666	137	1.31	0.40
TlNbO2F	1:4:-2:-1	0.99	3.39	-6.845	-2.37	186	ce01666	93	0.00	0.00
TlOsO2F	1:4:-2:-1	1.01	3.42	-6.119	-1.42	186	ce01402	114	0.00	0.04
TlSbO2F				-4.970	-1.69	241	ce00563	138	1.74	0.00
TlSnO2F	1:4:-2:-1	0.98	3.39	-5.064	-1.81	256	icsd84635a	165	1.32	0.00
TlTeO2F	1:4:-2:-1	0.87	3.90	-4.557	-1.47	222	ce00563	44	2.64	0.00
TlTiO2F	1:4:-2:-1	1.03	3.45	-6.705	-2.67	228	icsd84635a	12	3.09	0.00
TlWO2F	1:4:-2:-1	1.00	3.40	-5.963	-1.79	178	icsd68098a	159	1.75	0.40
TlZrO2F	1:4:-2:-1	0.97	3.39	-7.087	-2.92	164	ce00112	68	3.14	0.00

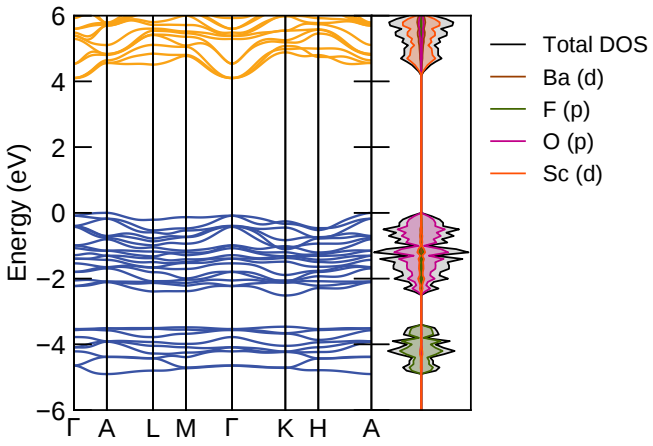
composition	oxidation state	t	tau	Spacegroup 123			Prototypes			
				E_total (eV)	E_form (eV/atom)	E_hull (meV/atom)	structure	E_hull (meV/atom)	Gap (eV)	Magnetization
LaMgF2N	3:2:-1:-3	0.81	5.64	-6.225	-2.76	155	icsd84635a	19	2.26	0.00



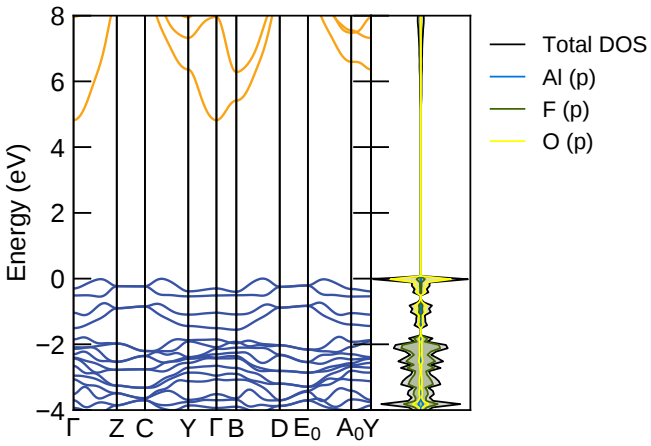
(a) $SrTaO_2N$



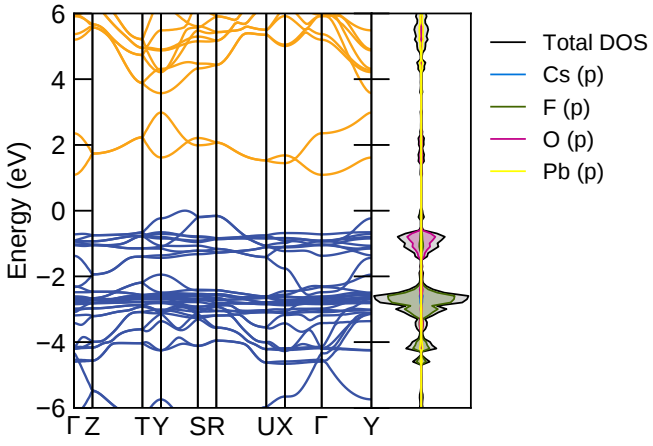
(b) $CaReO_2N$



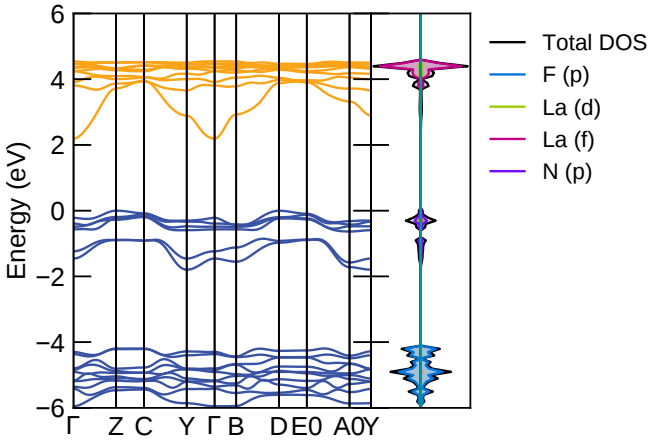
(c) $BaScO_2F$



(d) $NaAlF_2O$



(e) $CsPbF_2O$



(f) $LaMgF_2N$

FIG. S1: The band structures and density of electronic states (DOS) of the lowest energy perovskite structures calculated with PBE for (a) $SrTaO_2N$, (b) $CaReO_2N$, (c) $BaScO_2F$, (d) $NaAlF_2O$, (e) $CsPbF_2O$, and (f) $LaMgF_2N$.