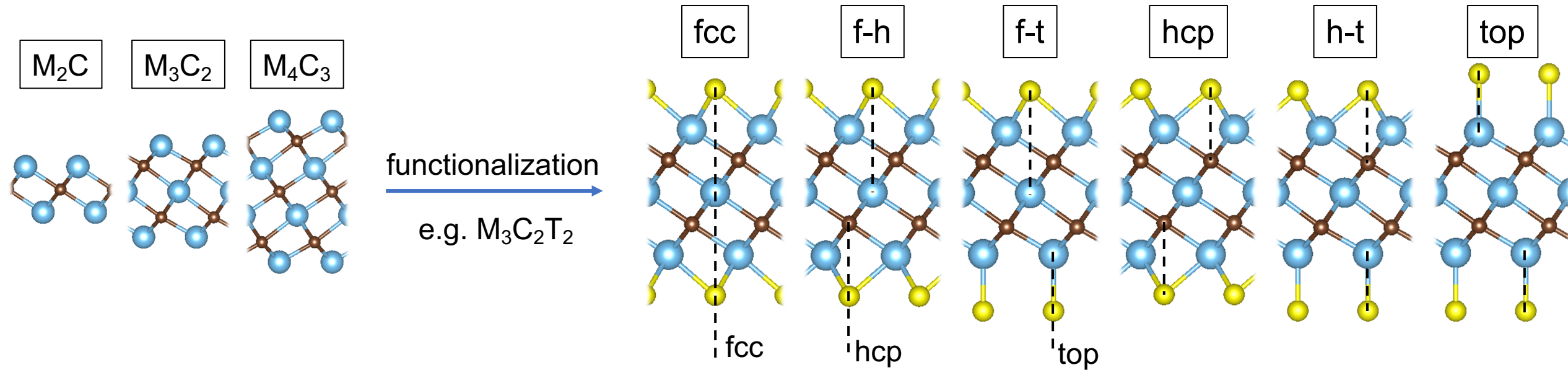


Configurations



5-f-h-3.02-1y-1Y

reference 5 – model f-h – lattice parameter $a=3.02$ – phonon spectrum: stable – molecular dynamic: stable

0-fcc-3.254 (in red: calculated by myself)

0 (from my calculation) – model fcc – lattice parameter $a=3.254$

M_{n+1}C_nT₂

	n	Sc	Ti	V	Cr	Zr	Nb	Mo	Hf	Ta	W
bare	1	1-3.313	32-3.01-1y	37-2.775-1y-1Y	37-2.659-1y-1Y	31-3.280-1y	27-3.112-1y	23-2.85-1y-1Y	1-3.193	27-3.075-1y	24-2.857-1y
	2	0-3.359	2-3.071	0-2.947	0-2.823	31-3.359-1y	10-3.139	0-3.016	0-3.265	2-3.196	0-2.987
	3	0-3.399	2-3.066	0-2.916	0-2.864	31-3.352-1y	0-3.132	0-3.080	0-3.284	2-3.172	0-3.083
OH	1	21-fcc-3.305-1y	3-fcc-3.072	25-fcc-3.00-1y	3-fcc-3.040	31-fcc-3.324-1y	3-fcc-3.195	3-fcc-3.284	3-fcc-3.264	3-fcc 0-hcp-3.026	3-fcc 0-hcp-2.967
	2	0-fcc-3.254	12-fcc-3.071	0-hcp-2.886	0-hcp-2.827	31-fcc-3.349-1y	10-hcp-2.990	0-hcp-3.031	8-fcc-3.30	0-hcp-3.081	0-hcp-2.996
	3	0-fcc-3.270	0-fcc-3.092	0-hcp-2.901	0-fcc-2.942	31-fcc-3.356-1y	12-fcc 0-hcp-3.018	0-hcp-3.061	0-fcc-3.296	0-hcp-3.104	0-top-3.136
F	1	21-fcc-3.281-1y	3-fcc-3.057	25-fcc-2.99-1y	3-fcc-3.022	31-fcc-3.312-1y	28-fcc-3.197-1y-1Y	3-fcc-3.264	3-fcc-3.247	3-fcc-3.195	3-top-3.071
	2	0-fcc-3.234	18-fcc-3.071-1y-1Y	0-hcp-2.857	0-top-2.967	31-fcc-3.344-1y	10-hcp-2.972	0-top-3.124	8-fcc-3.29	0-hcp-3.061	0-top-3.054
	3	0-fcc-3.253	0-fcc-3.084	0-fcc-2.942	0-top-2.939	31-fcc-3.354-1y	0-fcc-3.202	0-top-3.135	0-fcc-3.292	0-hcp-3.088	0-top-3.125
Cl	1	6-fcc-3.42-1y	6-fcc-3.23-1y	6-fcc-3.16-1n	6-fcc-3.17-1n	6-fcc-3.44-1y	6-fcc-3.33-1y	6-fcc-3.37-1n	6-fcc-3.40-1y	6-fcc-3.32-1y	6-fcc-3.38-1n
	2	6-fcc-3.37-1y	18-fcc-3.19-1y-1Y	6-fcc-3.13-1n	6-fcc-3.12-1n	6-fcc-3.42-1y	6-hcp-3.19-1y	6-hcp-3.14-1n	6-fcc-3.37-1y	6-hcp-3.17-1y	6-top-3.13-1n
	3	0-fcc-3.367	0-fcc-3.168	0-fcc-3.026	0-fcc-3.016	0-fcc-3.400	0-fcc-3.254	0-fcc-3.196	0-fcc-3.357	0-hcp-3.162	0-top-3.160
Br	1	0-fcc-3.509	0-fcc-3.322	0-fcc-3.283	0-fcc-3.257	0-fcc-3.511	0-fcc-3.453	4-fcc-fcc-3.417	0-fcc-3.468	0-fcc-3.448	0-fcc-3.432
	2	0-fcc-3.437	15-fcc-3.252	0-fcc-3.198	0-fcc-3.181	0-fcc-3.457	0-f-h-3.241	0-fcc-3.377	0-fcc-3.416	0-hcp-3.211	0-top-3.179
	3	0-fcc-3.411	0-fcc-3.218	0-fcc-3.081	0-top-3.004	0-fcc-3.435	0-fcc-3.285	0-fcc-3.232	0-fcc-3.390	0-hcp-3.204	0-top-3.181
I	1	0-fcc-3.648	0-fcc-3.469	0-fcc-3.431	0-fcc-3.394	0-fcc-3.634	0-fcc-3.573	0-fcc-3.539	0-fcc-3.596	0-fcc-3.569	0-fcc-3.552
	2	0-fcc-3.492	15-fcc-3.357	0-fcc-3.295	0-top-3.180	0-fcc-3.541	0-fcc-3.501	0-top-3.265	0-fcc-3.502	0-fcc-3.437	0-top-3.242
	3	0-fcc-3.469	0-fcc-3.305	0-fcc-3.192	0-top-3.110	0-fcc-3.498	0-fcc-3.381	0-top-3.224	0-fcc-3.458	0-hcp-3.273	0-top-3.216
O	1	29-f-h-3.44-1y	19-fcc-3.04-1y-1Y	3-fcc 25-f-h-2.99-1y	26-fcc- -1y 0-hcp-2.692	31-fcc-3.319-1y	3-fcc-3.131	26-fcc- -1y 0-hcp-2.882	22-fcc-3.266-1y	34-fcc-3.128-1y	3-hcp-2.878 26-fcc- -1y
	2	7-fcc-3.04-1Y	18-fcc-3.12-1y-1Y	14-fcc-2.910	14-fcc 0-hcp-2.738	31-fcc-3.323-1y	10-fcc 0-f-h-3.075	14-hcp-2.930	8-fcc-3.27	14-fcc-3.139	14-hcp-2.910
	3	14-hcp-3.431	14-fcc-3.045	14-fcc-2.914	14-hcp	31-fcc-3.324-1y	12-fcc-3.145	14-hcp-2.986	14-fcc-3.265	14-fcc-3.145	14-hcp-2.940
S	1	5-f-h-3.27-1n	5-fcc-3.19-1n 19-fcc- -1y-1Y	5-fcc-3.06-1y-1Y	5-hcp-2.93-1y-1Y	5-fcc-3.48-1n 35-fcc-3.477-1y	5-f-h-3.27-1y-1Y	5-hcp-3.08-1n 35-hcp-3.077-1y	5-fcc-3.42-1y-1Y	5-f-h-3.26-1y-1Y	5-hcp-3.06-1n 35-hcp-3.068-1y
	2	7-fcc-3.15-1Y	18-fcc-3.148-1y-1Y	0-fcc-3.040	0-hcp-2.913	0-fcc-3.420	0-hcp-3.157	0-hcp-3.085	0-fcc-3.375	0-fcc-3.250	0-hcp-3.073
	3	0-hcp-3.650	0-fcc-3.124	0-fcc-2.997	0-hcp-2.904	0-fcc-3.396	0-hcp-3.148	0-hcp-3.095	0-fcc-3.352	0-hcp-3.197	0-hcp-3.096
Se	1	0-fcc-3.320	0-fcc-3.236	33-fcc-3.122-1y	0-fcc-3.120	0-fcc-3.492	0-f-h-3.320	0-hcp-3.151	0-fcc-3.452	0-f-h-3.318	0-hcp-3.137
	2	7-fcc-3.17-1Y	0-fcc-3.172	0-fcc-3.094	0-hcp-2.972	0-fcc-3.423	0-hcp-3.206	0-hcp-3.132	0-fcc-3.380	0-fcc-3.313	0-hcp-3.129
	3	0-fcc-3.294	0-fcc-3.147	0-fcc-3.033	0-hcp-2.955	0-fcc-3.397	0-hcp-3.188	0-hcp-3.130	0-fcc-3.354	0-hcp-3.220	0-hcp-3.129
Te	1	0-fcc-3.412	0-fcc-3.305	33-fcc-3.252-1y	0-fcc-3.235	0-fcc-3.511	0-fcc-3.413	0-fcc-3.398	0-fcc-3.479	0-fcc-3.427	0-fcc-3.439
	2	7-fcc-3.24-1Y	0-fcc-3.233	0-fcc-3.191	0-fcc-3.166	0-fcc-3.439	0-hcp-3.279	0-f-h-3.233	0-fcc-3.406	0-fcc-3.366	0-f-h-3.235
	3	0-fcc-3.342	0-fcc-3.203	0-fcc-3.124	0-fcc-3.063	0-fcc-3.419	0-fcc-3.287	0-fcc-3.218	0-fcc-3.382	0-hcp-3.268	0-fcc-3.225

M_{n+1}N_nT₂

	n	Sc	Ti	V	Cr	Zr	Nb	Mo	Hf	Ta	W
bare	1	0-3.163	32-2.95-1y	36-3.095-1y-1Y	30-2.660-1Y	0-3.226	0-3.122	0-2.782	0-3.157	0-3.078	0-2.756
	2	0-3.183	0-3.034	0-2.850	0-2.871	0-3.179	0-3.067	0-3.083	0-3.134	0-3.041	0-3.029
	3	0-3.196	13-2.9915	0-2.929	0-2.730	0-3.233	0-3.159	0-2.798	0-3.181	0-3.138	0-2.780
OH	1	0-fcc-3.200	16-fcc-3.067	17-fcc-3.046	30-fcc-3.045-1Y	16-fcc-3.302	0-hcp-2.985	0-fcc-3.280	16-hcp-3.121	0-hcp-2.965	0-fcc-3.321
	2	0-fcc-3.196	0-hcp-2.972	0-hcp-2.828	0-fcc-2.967	0-fcc-3.329	0-hcp-2.990	0-fcc-3.203	0-hcp-3.151	0-hcp-2.965	0-f-h-2.807
	3	0-fcc-3.193	20-f-h 0-fcc-3.028	0-fcc-2.988	0-fcc-3.004	0-fcc-3.334	0-hcp-3.018	0-fcc-3.242	0-hcp-3.167	0-hcp-2.973	0-f-h-2.805
F	1	0-fcc-3.173	16-fcc-3.066	17-fcc-3.043	30-fcc-3.029-1Y	16-fcc-3.275	0-fcc-3.257	0-fcc-3.269	16-hcp-3.074	0-hcp-2.949	0-top-2.842
	2	0-fcc-3.179	11-hcp-2.942-1y	0-hcp-2.798	0-fcc-2.951	11-hcp-3.173-1y	0-hcp-2.972	9-fcc-3.35-1y-1Y 0-f-t-3.172	11-hcp-3.124-1y	0-hcp-2.941	0-top-2.827
	3	0-fcc-3.182	13-fcc-3.025	0-fcc-2.982	0-fcc-2.995	0-hcp-3.189	0-fcc-3.202	0-fcc-3.235	0-hcp-3.137	0-hcp-2.959	0-top-2.820
Cl	1	6-fcc-3.35-1y	6-fcc-3.24-1n	6-fcc-3.21-1n	6-fcc-3.17-1n	6-fcc-3.44-1y	6-fcc-3.41-1n	6-fcc-3.35-1n	6-fcc-3.40-1y	6-fcc-3.40-1n	6-fcc-3.39-1n
	2	6-fcc-3.30-1y	6-fcc-3.20-1y	6-fcc-3.05-1n	6-fcc-3.12-1n	6-hcp-3.34-1y	6-fcc-3.19-1n	6-fcc-3.24-1n	6-hcp-3.28-1y	6-fcc-3.16-1n 0-hcp-3.102	6-f-t-3.21-1n
	3	0-fcc-3.270	0-fcc-3.112	0-fcc-3.058	fcc-3.058	0-hcp-3.276	0-fcc-3.254	0-fcc-3.276	0-hcp-3.231	0-hcp-3.120	0-fcc-3.300
Br	1	0-fcc-3.437	0-fcc-3.322	0-fcc-3.288	fcc-3.260	0-fcc-3.502	0-fcc-3.468	0-fcc-3.403	0-fcc-3.460	0-fcc-3.465	0-fcc-3.464
	2	0-fcc-3.356	0-fcc-3.253	0-fcc-3.229	fcc-3.171	0-hcp-3.340	0-f-h-3.241	0-fcc-3.303	0-hcp-3.289	0-hcp-3.200	0-f-t-3.269
	3	0-fcc-3.316	0-fcc-3.171	0-fcc-3.113	fcc-3.098	0-hcp-3.320	0-fcc-3.285	0-fcc-3.303	0-hcp-3.274	0-fcc-3.294	0-fcc-3.327
I	1	0-fcc-3.589	0-fcc-3.469	0-fcc-3.419	fcc-3.383	0-fcc-3.627	0-fcc-3.573	0-fcc-3.557	0-fcc-3.588	0-fcc-3.575	0-fcc-3.592
	2	0-fcc-3.468	0-fcc-3.357	0-fcc-3.308	top-3.211	0-hcp-3.466	0-fcc-3.501	0-fcc-3.441	0-hcp-3.423	0-fcc-3.502	0-f-t-3.106
	3	0-fcc-3.403	0-fcc-3.252	0-fcc-3.194	top-3.172	0-f-h-3.423	0-fcc-3.381	0-fcc-3.361	0-hcp-3.365	0-fcc-3.388	0-top-3.311
O	1	14-fcc-3.224	14-fcc-3.001	14-fcc-2.906	14-hcp-2.669 30-fcc- -1y-1Y	14-fcc-3.250	14-fcc 0-hcp-2.989	14-hcp-2.872	14-fcc-3.210	14-fcc 0-hcp-2.985	14-hcp-2.869
	2	14-fcc-3.218	14-fcc-3.012	14-fcc-2.904	14-fcc 0-hcp-2.680	14-fcc-3.253	14-fcc 0-f-h-3.075	14-hcp-2.850	14-fcc-3.213	14-hcp 0-f-h-3.073	14-hcp-2.840
	3	14-fcc-3.211	13-fcc-3.008	14-fcc-2.905	14-hcp-2.693	14-fcc-3.248	14-fcc-3.145	14-hcp-2.835	14-fcc-3.206	14-hcp-3.027	14-hcp-2.824
S	1	5-fcc-3.33-1n	5-fcc-3.17-1n	5-fcc-3.08-1n	5-f-h-3.02-1y-1Y 0-hcp-2.902	5-fcc-3.44-1n	5-hcp-3.31-1n	5-hcp-3.34-1n	5-fcc-3.39-1n	5-hcp-3.15-1n	5-hcp-3.04-1n
	2	0-fcc-3.262	0-fcc-3.131	0-hcp-2.957	0-hcp-2.865	0-fcc-3.388	0-hcp-3.157	0-hcp-2.997	0-fcc-3.341	0-hcp-3.153	0-hcp-2.973
	3	0-fcc-3.238	0-fcc-3.094	0-hcp-2.944	0-hcp-2.852	0-fcc-3.343	0-hcp-3.148	0-hcp-3.141	0-fcc-3.302	0-hcp-3.146	0-hcp-3.153
Se	1	0-fcc-3.349	0-fcc-3.232	0-fcc-3.127	0-fcc-3.138	0-fcc-3.486	0-fcc-3.351	0-hcp-3.120	0-fcc-3.447	0-fcc-3.371	0-hcp-3.111
	2	0-fcc-3.268	0-fcc-3.169	0-f-h-3.034	0-f-h-3.030	0-fcc-3.415	0-hcp-3.206	0-f-h-3.240	0-fcc-3.378	0-hcp-3.203	0-f-h-3.256
	3	0-fcc-3.240	0-fcc-3.120	0-fcc-3.031	0-fcc-3.042	0-fcc-3.364	0-hcp-3.188	0-hcp-3.178	0-fcc-3.325	0-hcp-3.184	0-f-h-3.201
Te	1	0-fcc-3.409	0-fcc-3.311	0-fcc-3.257	0-fcc-3.234	0-fcc-3.504	0-fcc-3.426	0-fcc-3.418	0-fcc-3.479	0-fcc-3.447	0-fcc-3.466
	2	0-fcc-3.323	0-fcc-3.247	0-fcc-3.193	0-fcc-3.153	0-fcc-3.450	0-hcp-3.279	0-f-h-3.305	0-fcc-3.421	0-hcp-3.281	0-f-h-3.323
	3	0-fcc-3.289	0-fcc-3.169	0-fcc-3.098	0-fcc-3.095	0-fcc-3.365	0-fcc-3.287	0-fcc-3.313	0-fcc-3.332	0-hcp-3.254	0-f-t-3.039

Reference

			phonon spectrum	molecular dynamic
1	https://doi.org/10.1016/j.apsusc.2019.05.311	Applied Surface Science 488 (2019) 578–585	0 (without phonon spectrum)	0 (without MD)
2	10.1557/mrc.2012.25	MRS Communications (2012), 2, 133–137	0	0
3	10.1209/0295-5075/111/26007	EPL, 111 (2015) 26007	0	0
4	10.1039/c4cp00467a	Phys.Chem.Chem.Phys., 2014, 16, 7841	0	0
5	https://doi.org/10.1016/j.commatsci.2018.07.008	Computational Materials Science 153 (2018) 303–308	1 (with phonon spectrum)	1 (with MD)
6	https://doi.org/10.1088/1361-648X/ab6048	J. Phys.: Condens. Matter 32 (2020) 135302 (9pp)	1	0
7	https://doi.org/10.1016/j.apsusc.2019.144221	Applied Surface Science 501 (2020) 144221	0	1
8	10.1021/acsnano.7b00030	ACS Nano 2017, 11, 3841–3850	0	0
9	https://doi.org/10.1063/1.4993869	Appl. Phys. Lett. 111, 202405 (2017)	1	1
10	https://doi.org/10.1016/j.commatsci.2017.11.019	Computational Materials Science 143 (2018) 225–231	0	0
11	10.1103/PhysRevB.96.195414	PHYSICAL REVIEW B 96, 195414 (2017)	1	0
12	10.1021/acscatal.6b02754	ACS Catal. 2017, 7, 494–500	0	0
13	10.1039/c6nr02253g	Nanoscale, 2016, 8, 11385	0	0
14	10.1021/acs.chemmater.8b00156	Chem. Mater. 2018, 30, 2687–269	0	0
15	https://dx.doi.org/10.1021/acsnano.0c07972	ACS Nano 2021, 15, 1077–1085	0	0
16	10.1002/adfm.201202502	Adv. Funct. Mater. 2013, 23, 2185–2192	0	0
17	10.1021/acsnano.7b02578	ACS Nano 2017, 11, 7648–7655	0	0
18	10.1021/acsnano.9b03412	ACS Nano 2019, 13, 11078–11086	1	1
19	https://doi.org/10.1016/j.commatsci.2019.03.039	Computational Materials Science 163 (2019) 267–277	1	1
20	10.1039/c6nr02253g	Nanoscale, 2016, 8, 11385	0	0
21	10.1039/c5nr08639f	Nanoscale, 2016, 8, 6110	1	0
22	10.1038/srep27971	Sci. Rep. 6, 27971 (2016)	1	0
23	10.1021/acs.jpcclett.6b00171	J. Phys. Chem. Lett. 2016, 7, 937–943	1	1
24	10.1039/c8cp01353e	Phys. Chem. Chem. Phys., 2018, 20, 18924–18930	1	0
25	10.1103/PhysRevB.97.115439	PHYSICAL REVIEW B 97, 115439 (2018)	1	0
26	10.1103/PhysRevB.92.075436	PHYSICAL REVIEW B 92, 075436 (2015)	1	0
27	https://doi.org/10.1088/1361-648X/ab2847	J. Phys.: Condens. Matter 31 (2019) 405703 (12pp)	1	0
28	10.1039/c9ta12255a	J. Mater. Chem. A (2020)	1	1

			phonon spectrum	molecular dynamic
29	10.1021/acs.jpcc.7b06162	J. Phys. Chem. C 2017, 121, 18947–18953	1	0
30	10.1021/acs.jpcc.6b05224	J. Phys. Chem. C 2016, 120, 18850–18857	1	1
31	10.1088/0253-6102/69/3/336	Commun. Theor. Phys. 69 (2018) 336–342	1	0
32	10.1039/c7cp08270c	Phys.Chem.Chem.Phys., 2018, 20, 7754	1	0
33	https://doi.org/10.1039/D1QM00422K	Mater. Chem. Front., 2021, Advance Article	1	0
34	10.1021/acs.jpcc.8b00142	J. Phys. Chem. C 2018, 122, 4710–4722	1	0
35	https://dx.doi.org/10.1021/acs.jpcc.0c05287	J. Phys. Chem. C 2020, 124, 21293–21304	1	1
36	https://doi.org/10.1016/j.jcis.2021.03.018	Journal of Colloid and Interface Science 593 (2021) 51–58	1	1
37	10.1039/c7cp00064b	Phys. Chem. Chem. Phys., 2017, 19, 7807–7819	1	1