Supplementary to Magnetic i-MXene: a new class of multifunctional two-dimensional materials

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S1 Spin configuration

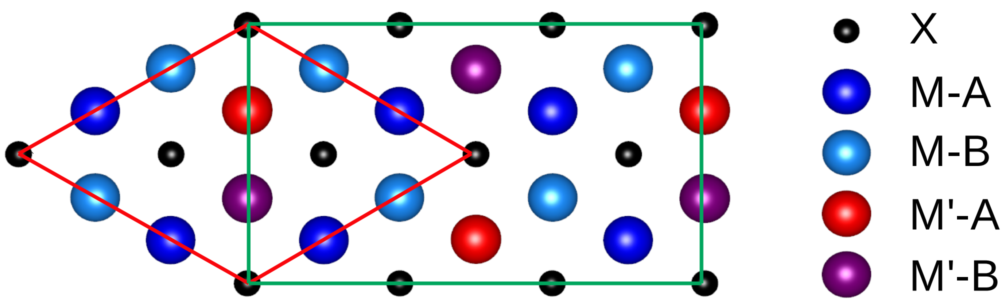


Figure S1: Crystal structure for i-MXene $(M_{2/3}M'_{1/3})_2X$ in hexagonal (red) and rectangular (green) lattices. The "A" and "B" symbols denote the corresponding atoms lie above and below the center layer X (X = C and N) atoms. In the following structures, the atom labels have the same meaning as this figure.

S2 Noncolinear spin configurations

In the hexagonal lattice, the doped transition metal M′ of intralayer forms a triangular lattice in the 2×2×1 super cell as showing in Fig. S3, implying the noncolinear antiferromagnetic state may be stable. Table S1 lists the noncolinear antiferromagnetic candidates.

Table S1: The noncolinaer antiferromagnetic candidates

spin	Candidate
AFM-β	$(Sc_{2/3}Mo_{1/3})_2C$ $(Nb_{2/3}Mn_{1/3})_2C$ $(Zr_{2/3}Mn_{1/3})_2C$ $(Sc_{2/3}Nb_{1/3})_2C$
AFM-α	$(Ta_{2/3}Mn_{1/3})_2C$ $(Mo_{2/3}Fe_{1/3})_2C$ $(Zr_{2/3}Ni_{1/3})_2C$ $(Zr_{2/3}Fe_{1/3})_2C$ $(Hf_{2/3}Mn_{1/3})_2C$ $(Zr_{2/3}Co_{1/3})_2N$ $(Ti_{2/3}Fe_{1/3})_2N$ $(Zr_{2/3}Mn_{1/3})_2N$ $(Zr_{2/3}Fe_{1/3})_2N$ $(V_{2/3}Mn_{1/3})_2C$ $(Hf_{2/3}Cr_{1/3})_2N$

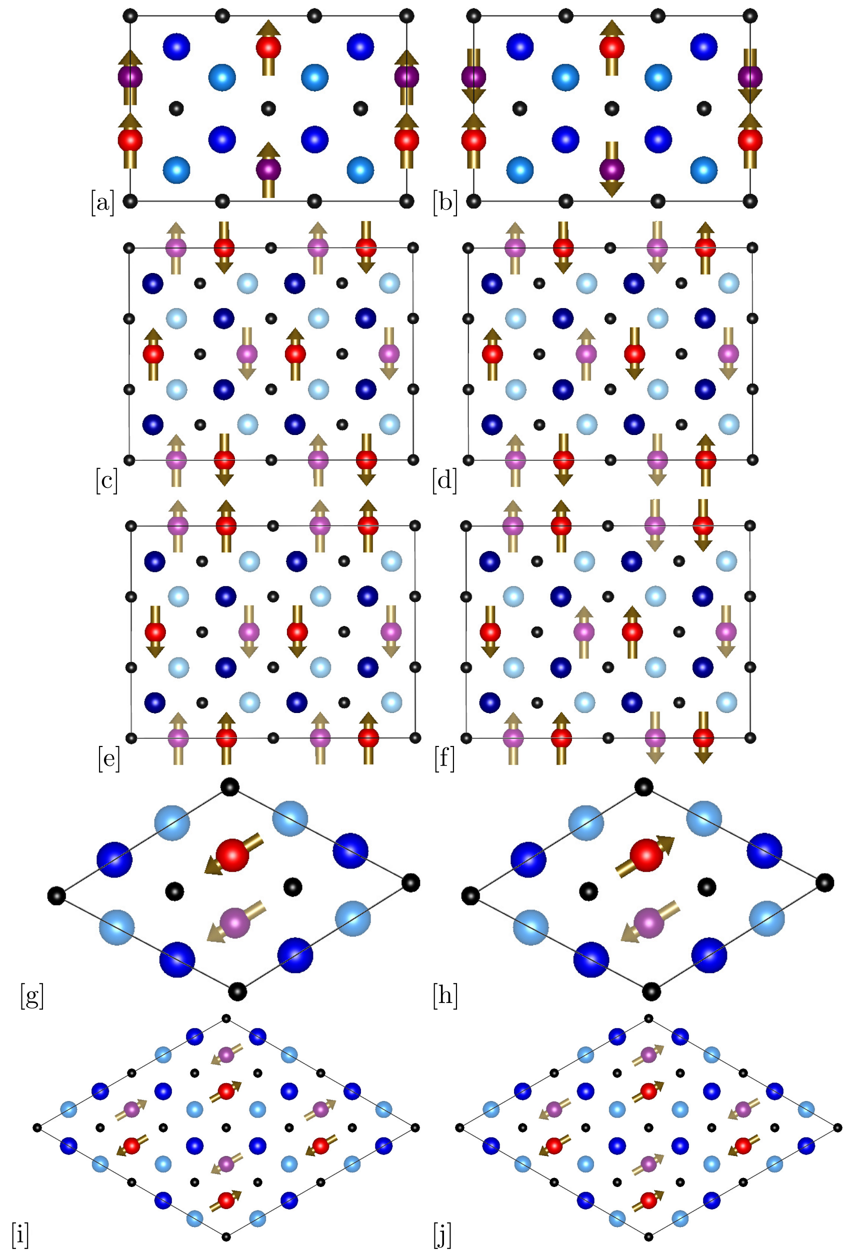
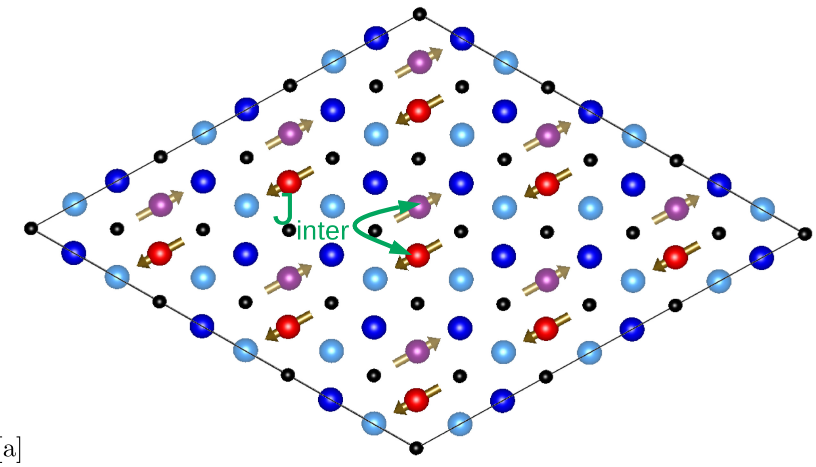
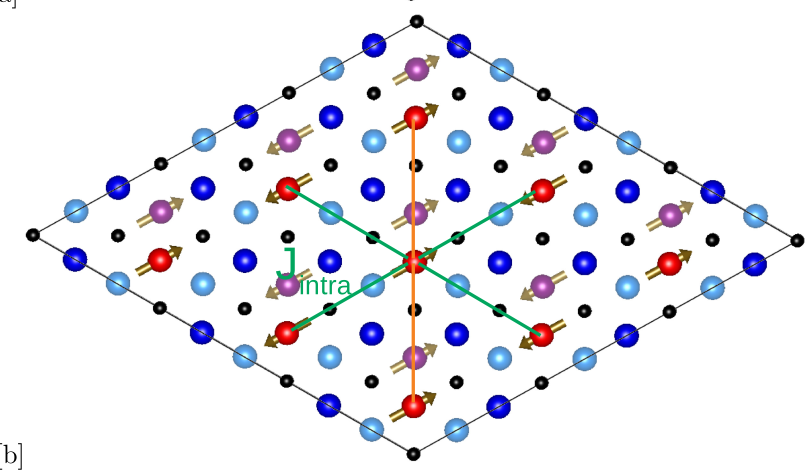


Figure S2: Spin configurations for i-MXene in rectangular lattice: [a] ferromagnetic (FM) and [b] interlayer antiferromagnetic (AFM-0) spin state. For comparison with hexagonal i-MXene in noncolinear spin configuration, we also calculate rectangular i-MXene in similar spin configurations. [c] AFM-1 and [d] AFM-2 are the interlayer antiferromagnetic coupling spin configurations, while [e] AFM-3 and [f] AFM-4 are the interlayer ferromagnetic coupling spin configurations. Noncolinear antiferromagnetic spin configurations for the interlayer coupling of antiferromagnetic (AFM-α) [i] and ferromagnetic (AFM-β) [j] cases.



[a]



[b]

Figure S3: The schematic diagrams of exchange coupling parameters [a] J_{inter} and [b] J_{intra} for i-MXene $(Hf_{2/3}Fe_{1/3})_2C$. [a] AFM-0: The exchange coupling of Fe atoms of above and below layers is set as antiferromagnetic, while the intralayer coupling for Fe is set as ferromagnetic. [b] AFM-β: The intralayer coupling of Fe atoms is set as noncolinear antiferromagnetic while the interlayer coupling of Fe atoms are ferromagnetic. It should be noticed there are in total 6 nearest neighbor Fe atoms for each Fe, of which four are antiferromagnetic and two are ferromagnetic to the center of Fe atom of the hexagonal Fe atoms.

S3 DOS for some i-MXene.

In order to discuss i-MXene with spin configuration transition from NM to FM, we have shown the density of states (DOS) for $(Zr_{2/3}Ti_{1/3})_2N$, $(Ti_{2/3}Ru_{1/3})_2C$ and $(Zr_{2/3}Ru_{1/3})_2C$ in Fig. S4. We also show the Fe atomic DOS in $(Hf_{2/3}Fe_{1/3})_2C$ with the hexagonal and rectangular lattice in order to understand the spin configuration transition from AFM to FM.

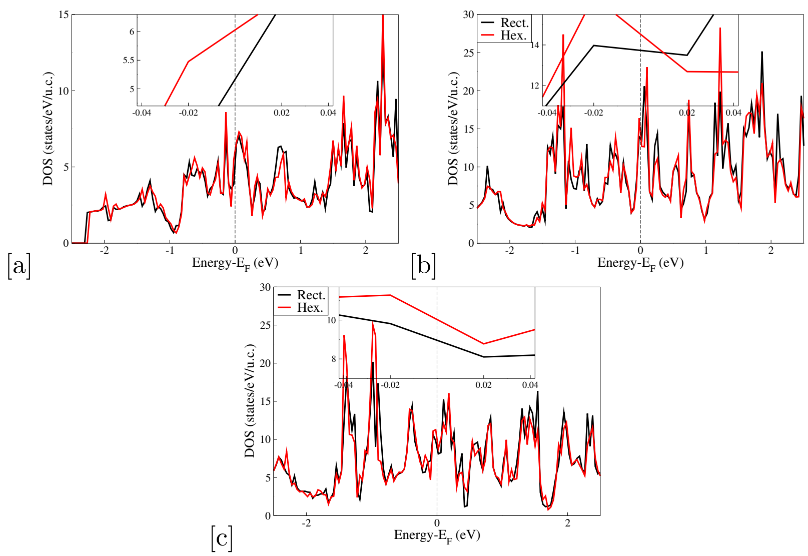


Figure S4: Density of states comparison between rectangular (Rect.) and hexagonal (Hex.) lattices for [a] $(Zr_{2/3}Ti_{1/3})_2N$, [b] $(Ti_{2/3}Ru_{1/3})_2C$ and [c] $(Zr_{2/3}Ru_{1/3})_2C$ in non-magnetic spin configuration.

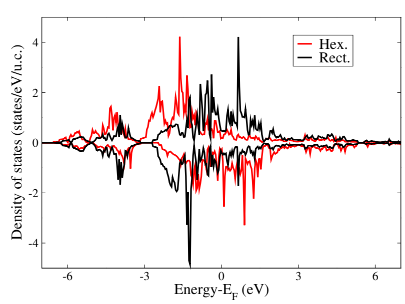


Figure S5: Fe atomic DOS in $(Hf_{2/3}Fe_{1/3})_2C$ withe hexagonal and rectangular lattice.

S4 Band structures and AHC for $(Ti_{2/3}V_{1/3})_2C$.

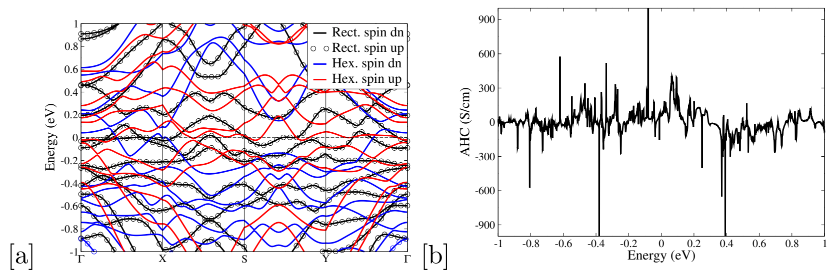


Figure S6: [a] Band structures for $(Ti_{2/3}V_{1/3})_2C$ in rectangular (Rect.) and hexagonal (Hex.) lattices. In rectangular lattice, the band structures of spin up and spin down (dn) are overlapping. For the hexagonal lattice, here we use the $k-$path of rectangular lattice for comparison. [b] Anomalous hall conductivity for $(Ti_{2/3}V_{1/3})_2C$ in the hexagonal lattice.

S5 DOS and Seebeck coefficients for $(Sc_{2/3}Cd_{1/3})_2C$ and $(Sc_{2/3}Hg_{1/3})_2C$.

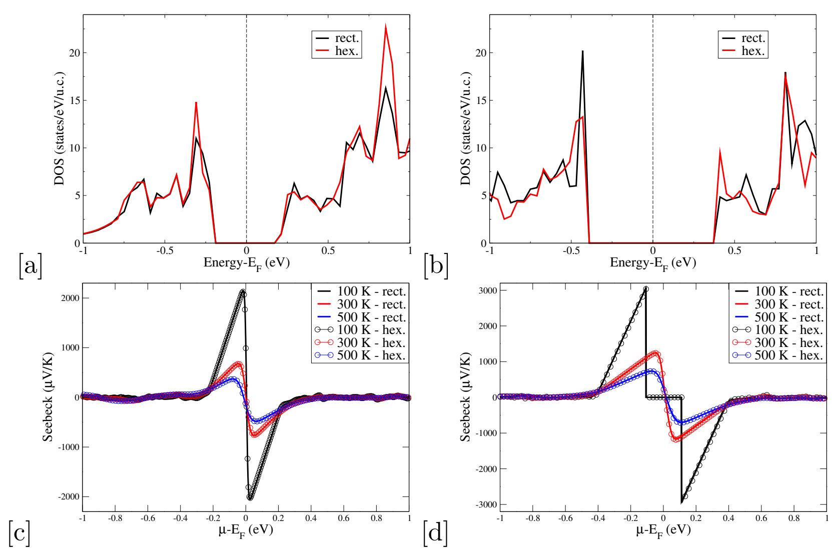
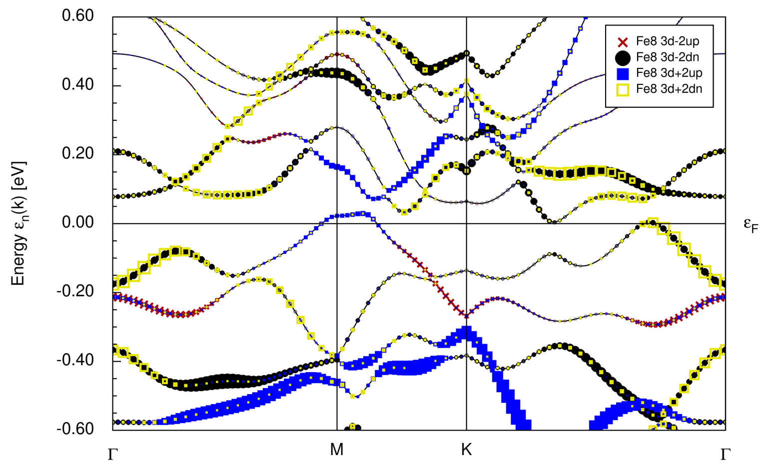
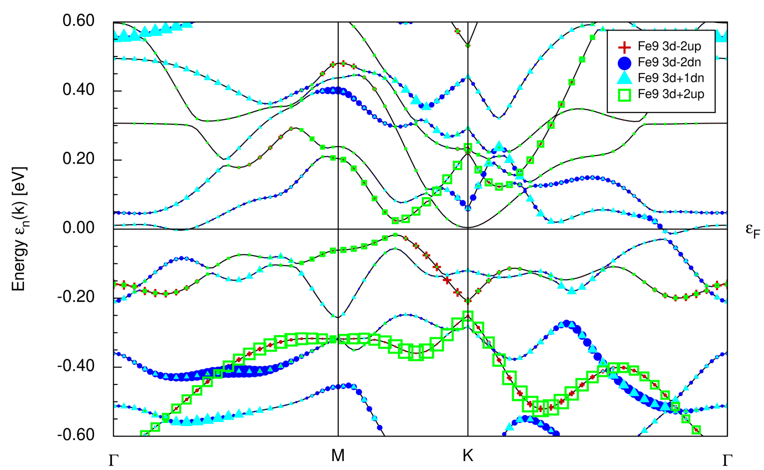


Figure S7: DOS for $(Sc_{2/3}Cd_{1/3})_2C$ [a] and $(Sc_{2/3}Hg_{1/3})_2C$ [b]. Seebeck coefficient as a function of chemical potential for $(Sc_{2/3}Cd_{1/3})_2C$ [a] and $(Sc_{2/3}Hg_{1/3})_2C$ [b]. The "rect." and "hex." denote the results in rectangular and hexagonal lattices.

S6 Projected band structures

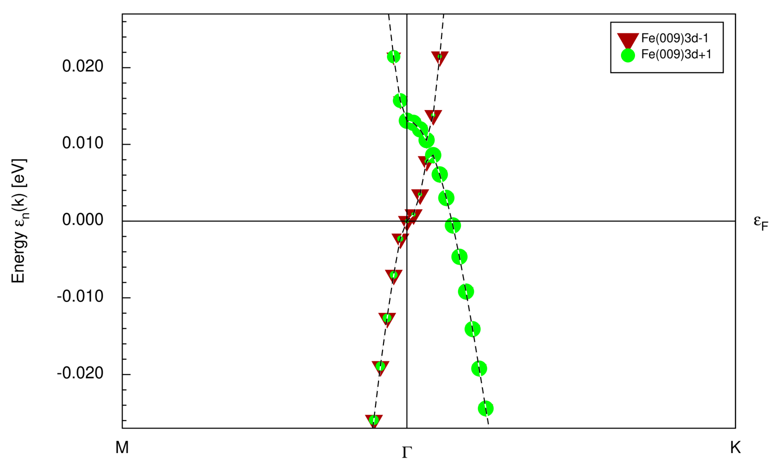


[a]

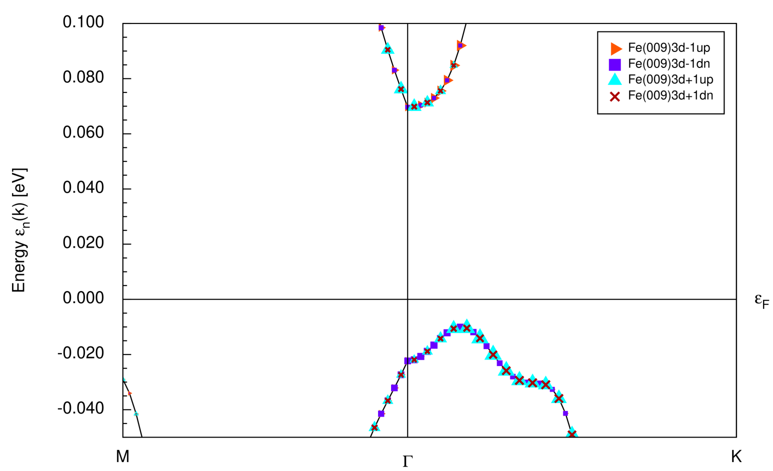


[b]

Figure S8: Orbital projected band structures for $(Hf_{2/3}Fe_{1/3})_2C$ (a) and $(Zr_{2/3}Fe_{1/3})_2C$. The Fe 3d-2 and Fe 3d+2 symbols denote the Fe 3d$_{xy}$ and Fe-3d$_{x^2-y^2}$ orbitals, respectively.



[a]



[b]

Figure S9: Orbital projected band structures for Fe atoms in $(Ta_{2/3}Fe_{1/3})_2C$ without and with SOC. The Fe 3d+1 and Fe 3d-1 symbols denote the Fe $3d_{zx}$ and Fe $3d_{yz}$ orbitals, respectively.

S7 MAE

Table S2: MAE values for i-MXene in hexagonal and rectangular lattices in unit of meV/f.u. $\Delta E = E_{hex.} - E_{rect.}$

Com.	hex	rect.	ΔE	Comp.	hex	rect.	ΔE
$(Hf_{2/3}Cr_{1/3})_2C$	0.092	0.0431	0.0489	$(Hf_{2/3}Fe_{1/3})_2C$	1.3854	1.4141	-0.0287
$(Hf_{2/3}Hg_{1/3})_2C$	-0.0001	-0.7499	0.7498	$(Hf_{2/3}Mn_{1/3})_2C$	-0.0567	-0.0979	0.0412
$(Mo_{2/3}Cr_{1/3})_2C$	0.0561	-0.0114	0.0675	$(Mo_{2/3}Fe_{1/3})_2C$	-0.0558	-0.0018	-0.054
$(Mo_{2/3}Mn_{1/3})_2C$	0.0109	-0.0319	0.0428	$(Nb_{2/3}Co_{1/3})_2C$	0.0158	-0.041	0.0568
$(Nb_{2/3}Fe_{1/3})_2C$	0.0286	0.0253	0.0033	$(Nb_{2/3}Mn_{1/3})_2C$	0.201	0.1018	0.0992
$(Nb_{2/3}Sc_{1/3})_2C$	0.0001	0.0	0.0001	$(Sc_{2/3}Cr_{1/3})_2C$	0.0775	0.0005	0.077
$(Sc_{2/3}Mn_{1/3})_2C$	0.0357	0.0159	0.0198	$(Sc_{2/3}Mo_{1/3})_2C$	0.0042	0.0	0.0042
$(Sc_{2/3}Nb_{1/3})_2C$	-0.0001	-0.0007	0.0006	$(Sc_{2/3}Ta_{1/3})_2C$	0.001	0.0665	-0.0655
$(Sc_{2/3}V_{1/3})_2C$	-0.009	0.0024	-0.0114	$(Ta_{2/3}Co_{1/3})_2C$	0.3184	0.2116	0.1068
$(Ta_{2/3}Fe_{1/3})_2C$	0.8628	0.3584	0.5044	$(Ta_{2/3}Mn_{1/3})_2C$	-0.0442	0.0868	-0.131
$(Ta_{2/3}Nb_{1/3})_2C$	0.0	-0.0001	0.0001	$(Ti_{2/3}Cr_{1/3})_2C$	0.0015	-0.0015	0.003
$(Ti_{2/3}Mo_{1/3})_2C$	0.0339	0.0253	0.0086	$(Ti_{2/3}Nb_{1/3})_2C$	0.0193	0.0254	-0.0061
$(Ti_{2/3}Pd_{1/3})_2C$	-0.0211	-0.0051	-0.016	$(Ti_{2/3}Sc_{1/3})_2C$	-0.0005	0.0023	-0.0028
$(Ti_{2/3}Ta_{1/3})_2C$	0.0565	-0.0093	0.0658	$(Ti_{2/3}V_{1/3})_2C$	0.0216	0.0195	0.0021
$(Ti_{2/3}Y_{1/3})_2C$	0.038	0.0083	0.0297	$(V_{2/3}Co_{1/3})_2C$	-0.0124	-0.0467	0.0343
$(V_{2/3}Fe_{1/3})_2C$	0.0535	0.0667	-0.0132	$(V_{2/3}Mn_{1/3})_2C$	0.0993	0.1013	-0.002
$(V_{2/3}Rh_{1/3})_2C$	-0.0505	-0.0708	0.0203	$(V_{2/3}Sc_{1/3})_2C$	-0.0128	0.0016	-0.0144
$(V_{2/3}Ti_{1/3})_2C$	0.0057	0.0059	-0.0002	$(Zr_{2/3}Cr_{1/3})_2C$	0.0056	0.0349	-0.0293
$(Zr_{2/3}Fe_{1/3})_2C$	0.7446	0.8125	-0.0679	$(Zr_{2/3}Hf_{1/3})_2C$	-0.6085	-0.0467	-0.5618
$(Zr_{2/3}Mn_{1/3})_2C$	0.0688	0.132	-0.0632	$(Zr_{2/3}Ni_{1/3})_2C$	0.0587	0.0348	0.0239
$(Hf_{2/3}Co_{1/3})_2N$	0.1272	0.1094	0.0178	$(Hf_{2/3}Cr_{1/3})_2N$	0.7536	0.6041	0.1495
$(Hf_{2/3}Fe_{1/3})_2N$	0.3874	-0.5089	0.8963	$(Hf_{2/3}Mn_{1/3})_2N$	-0.4437	-0.5283	0.0846
$(Hf_{2/3}Sc_{1/3})_2N$	-0.6875	-1.0708	0.3833	$(Hf_{2/3}Zr_{1/3})_2N$	0.054	0.0934	-0.0394
$(Ti_{2/3}Fe_{1/3})_2N$	-0.1369	-0.1276	-0.0093	$(Ti_{2/3}Hf_{1/3})_2N$	0.7144	0.4739	0.2405
$(Ti_{2/3}Mn_{1/3})_2N$	0.0735	0.0024	0.0711	$(Ti_{2/3}Nb_{1/3})_2N$	-0.0157	0.0496	-0.0653
$(Ti_{2/3}Sc_{1/3})_2N$	0.0026	0.002	0.0006	$(Ti_{2/3}V_{1/3})_2N$	0.0029	0.0049	-0.002
$(Ti_{2/3}Y_{1/3})_2N$	-0.021	0.0029	-0.0239	$(Zr_{2/3}Co_{1/3})_2N$	-0.0404	-0.0613	0.0209
$(Zr_{2/3}Fe_{1/3})_2N$	-0.0638	-0.0768	0.013	$(Zr_{2/3}Hf_{1/3})_2N$	0.0558	-0.1121	0.1679
$(Zr_{2/3}Mn_{1/3})_2N$	0.056	0.0532	0.0028	$(Zr_{2/3}Sc_{1/3})_2N$	0.0	0.0454	-0.0454
$(Zr_{2/3}V_{1/3})_2N$	0.0252	0.0145	0.0107	$(Ti_{2/3}Ti_{1/3})_2C$	0.0063	0.0	0.0063
$(Ti_{2/3}Ti_{1/3})_2N$	-0.0223	0.0	-0.0223				

S8 Energy comparison for Hexagonal and rectangular lattice

Table S3: The energy comparison for i-MXene in NM and FM spin configurations within hexagonal and rectangular lattice. E_{NM} and E_{FM} denote the energy of NM and FM spin configurations in unit of eV/atom. M_{tot} is the total magnetic moment in unit of $\mu_B/f.u.$

	Rect.			Hex.		
commpound	E_{NM}	E_{FM}	M_{tot}	E_{NM}	E_{FM}	M_{tot}
$(Hf_{2/3}Cr_{1/3})_2C$	0.0034	0.0	0.4118	0.0034	0.0	0.4293
$(Hf_{2/3}Hg_{1/3})_2C$	0.0022	0.0	0.2573	0.0005	0.0	0.344
$(Mo_{2/3}Cr_{1/3})_2C$	0.0085	0.0	0.8835	0.0109	0.0	0.842
$(Mo_{2/3}Fe_{1/3})_2C$	0.0452	0.0	1.182	0.044	0.0	1.173
$(Mo_{2/3}Mn_{1/3})_2C$	0.0588	0.0	1.2948	0.0594	0.0	1.318
$(Nb_{2/3}Co_{1/3})_2C$	0.0039	0.0	0.4637	0.0039	0.0	0.4497
$(Nb_{2/3}Fe_{1/3})_2C$	0.0283	0.0	1.0397	0.0288	0.0	1.0473
$(Ta_{2/3}Co_{1/3})_2C$	0.0053	0.0	0.4113	0.0058	0.0	0.453
$(Ta_{2/3}Mn_{1/3})_2C$	0.0283	0.0	0.7803	0.0283	0.0	0.7713
$(Ti_{2/3}Nb_{1/3})_2C$	0.0125	0.0	0.7057	0.0134	0.0	0.7147
$(Ti_{2/3}Pd_{1/3})_2C$	0.0041	0.0	0.3772	0.0049	0.0	0.382
$(Ti_{2/3}Sc_{1/3})_2C$	0.0093	0.0	0.8355	0.0113	0.0	0.836
$(Ti_{2/3}Ta_{1/3})_2C$	0.0112	0.0	0.725	0.0134	0.0	0.718
$(Ti_{2/3}Ti_{1/3})_2C$	0.0278	0.0	0.8935	0.0414	0.0	0.9207
$(V_{2/3}Co_{1/3})_2C$	0.0064	0.0	0.638	0.0073	0.0	0.6497
$(V_{2/3}Fe_{1/3})_2C$	0.0331	0.0	1.0948	0.0335	0.0	1.1273
$(V_{2/3}Mn_{1/3})_2C$	0.0277	0.0	0.697	0.0275	0.0	0.705
$(V_{2/3}Rh_{1/3})_2C$	0.0009	0.0	0.3035	0.0005	0.0	0.3033
$(Zr_{2/3}Cr_{1/3})_2C$	0.0034	0.0	0.3828	0.0034	0.0	0.425
$(Zr_{2/3}Fe_{1/3})_2C$	0.011	0.0	0.8817	0.0129	0.0	0.9173
$(Zr_{2/3}Ni_{1/3})_2C$	0.0033	0.0	0.3608	0.0032	0.0	0.336
$(Hf_{2/3}Co_{1/3})_2N$	0.0051	0.0	0.3463	0.0059	0.0	0.3637
$(Hf_{2/3}Cr_{1/3})_2N$	0.0012	0.0	0.2668	0.0016	0.0	0.3557
$(Hf_{2/3}Mn_{1/3})_2N$	0.035	0.0	0.7438	0.036	0.0	0.6857
$(Hf_{2/3}Zr_{1/3})_2N$	0.0025	0.0	0.5643	0.0031	0.0	0.5553
$(Ti_{2/3}Fe_{1/3})_2N$	0.0385	0.0	1.1135	0.0382	0.0	1.1017
$(Ti_{2/3}Hf_{1/3})_2N$	0.0035	0.0	0.5707	0.0043	0.0	0.5777
$(Ti_{2/3}Mn_{1/3})_2N$	0.0416	0.0	0.804	0.0413	0.0	0.8093
$(Ti_{2/3}Sc_{1/3})_2N$	0.0121	0.0	0.5993	0.0121	0.0	0.5753
$(Ti_{2/3}Ti_{1/3})_2N$	0.0003	0.0	0.5787	0.0144	0.0	0.575
$(Ti_{2/3}Y_{1/3})_2N$	0.002	0.0	0.3975	0.0016	0.0	0.3777
$(Zr_{2/3}Co_{1/3})_2N$	0.0094	0.0	0.4592	0.0101	0.0	0.469
$(Zr_{2/3}Fe_{1/3})_2N$	0.0341	0.0	1.235	0.0379	0.0	1.266
$(Zr_{2/3}Hf_{1/3})_2N$	0.0053	0.0	0.5257	0.0058	0.0	0.53
$(Zr_{2/3}Mn_{1/3})_2N$	0.0324	0.0	1.0635	0.034	0.0	1.07
$(Zr_{2/3}Y_{1/3})_2N$	0.0035	0.0	0.4002	0.0039	0.0	0.4207

Table S3: The energy comparison for i-MXene in NM and FM spin configurations within hexagonal and rectangular lattice. E_{NM} and E_{FM} denote the energy of NM and FM spin configurations in unit of eV/atom. M_{tot} is the total magnetic moment in unit of $\mu_B/f.u.$. (continued)

	Rect.			Hex.		
commpound	NM	FM	M_{tot}	NM	FM	M_{tot}
$(Nb_{2/3}Mn_{1/3})_2C$	0.0299	0.0	0.7793	0.0295	0.0	0.799
$(Nb_{2/3}Sc_{1/3})_2C$	0.0017	0.0	0.4298	0.0024	0.0	0.412
$(Sc_{2/3}Cr_{1/3})_2C$	0.0095	0.0	1.101	0.0066	0.0	1.1063
$(Sc_{2/3}Mn_{1/3})_2C$	0.0013	0.0	0.6163	0.0011	0.0	0.6443
$(Sc_{2/3}Mo_{1/3})_2C$	0.0008	0.0	0.8827	0.0048	0.0	0.731
$(Sc_{2/3}Nb_{1/3})_2C$	0.0028	0.0	0.4998	0.005	0.0	0.5507
$(Sc_{2/3}Ta_{1/3})_2C$	0.002	0.0	0.4267	0.0028	0.0	0.4363
$(Sc_{2/3}V_{1/3})_2C$	0.0	0.0	0.9322	0.0049	0.0	0.4447
$(Ta_{2/3}Fe_{1/3})_2C$	0.0237	0.0	1.0207	0.0249	0.0	1.0117
$(Ta_{2/3}Sc_{1/3})_2C$	0.0008	0.0	0.5032	0.0015	0.0	0.341
$(Ti_{2/3}Cr_{1/3})_2C$	0.001	0.0	0.2468	0.001	0.0	0.2323
$(Ti_{2/3}Mo_{1/3})_2C$	0.0019	0.0	0.2175	0.0022	0.0	0.2063
$(Ti_{2/3}Y_{1/3})_2C$	0.0039	0.0	0.7477	0.0002	0.0	0.2853
$(V_{2/3}Sc_{1/3})_2C$	0.0015	0.0	0.4797	0.0002	0.0	0.541
$(V_{2/3}Ti_{1/3})_2C$	0.0063	0.0	0.519	0.0019	0.0	0.4413
$(Zr_{2/3}Hf_{1/3})_2C$	0.0001	0.0	0.2242	0.0013	0.0	0.5593
$(Zr_{2/3}Mn_{1/3})_2C$	0.0026	0.0	0.7227	0.0041	0.0	0.714
$(Zr_{2/3}Y_{1/3})_2C$	0.0025	0.0	0.3045	0.002	0.0	0.666
$(Hf_{2/3}Fe_{1/3})_2N$	0.0321	0.0	1.0337	0.032	0.0	1.0477
$(Hf_{2/3}Sc_{1/3})_2N$	0.0065	0.0	0.4035	0.0009	0.0	0.6017
$(Ti_{2/3}Nb_{1/3})_2N$	0.0005	0.0	0.2492	0.0057	0.0	0.5223
$(Ti_{2/3}V_{1/3})_2N$	0.0011	0.0	0.2352	0.0	0.0	0.298
$(Zr_{2/3}Sc_{1/3})_2N$	0.0112	0.0	0.6917	0.0088	0.0	0.699
$(Hf_{2/3}Fe_{1/3})_2C$	0.0019	0.0	0.9	0.016	0.0	0.8797
$(Hf_{2/3}Mn_{1/3})_2C$	0.0068	0.0	0.525	0.0008	0.0	0.5257
$(Ti_{2/3}V_{1/3})_2C$	0.0053	0.0	0.722	0.0069	0.0	0.701

Table S4: The energy comparison for i-MXene with NM to FM spin configuration transition when the lattice is changed from hexagonal and rectangular.

commpound	NM	FM	AFM-0	AFM-β	AFM-α
$(Ti_{2/3}Ru_{1/3})_2C$	0.0007	0.0	0.0007	0.0007	0.0007
$(Zr_{2/3}Cu_{1/3})_2C$	0.0012	0.0	0.0012	0.0008	0.0012
$(Zr_{2/3}Ti_{1/3})_2N$	0.0015	0.0	0.0014	0.0016	0.0011

Table S5: Energy (in unit of eV/atom) compassion for i-MXene within various spin configurations in both rectangular (Rect.) and hexagonal (Hex.) lattice.

Compound	Structure	NM	FM	AFM-0	AFM-3 /AFM-β	AFM-2 /AFM-α	AFM-4	AFM-1
AFM→ FM								
$(Hf_{2/3}Fe_{1/3})_2C$	Rect.	0.016	0.0107	0.0	0.0018	0.0045	0.015	0.015
	Hex.	0.0105	0.0	0.0039	0.0021	0.0091	-	-
$(Hf_{2/3}Mn_{1/3})_2C$	Rect.	0.0084	0.0084	0.0050	0.0079	0.0	0.0147	0.0215
	Hex.	0.0119	0.0055	0.0089	0.0	0.0046	-	-
$(Ti_{2/3}V_{1/3})_2C$	Rect.	0.0069	0.0022	0.0	0.0055	0.0038	0.0062	0.0009
	Hex.	0.0042	0.0	0.002	0.0052	0.002	-	-
AFM→ AFM								
$(Nb_{2/3}Mn_{1/3})_2C$	Rect.	0.0408	0.0109	0.0076	0.0043	0.0	0.0069	0.0121
	Hex.	0.0361	0.0066	0.0031	0.0027	0.0	-	-
$(Nb_{2/3}Sc_{1/3})_2C$	Rect.	0.005	0.0033	0.0	0.0048	0.0043	0.0047	0.0043
	Hex.	0.0055	0.0031	0.0	0.0049	0.0054	-	-
$(Sc_{2/3}Cr_{1/3})_2C$	Rect.	0.0182	0.0087	0.0	0.0036	0.0156	0.0172	0.017
	Hex.	0.0184	0.0118	0.0	0.0176	0.0039	-	-
$(Sc_{2/3}Mn_{1/3})_2C$	Rect.	0.0079	0.0066	0.0016	0.0044	0.0011	0.0051	0.0
	Hex.	0.0089	0.0078	0.0	0.0039	0.0037	-	-
$(Sc_{2/3}Mo_{1/3})_2C$	Rect.	0.0023	0.0015	0.0	0.0031	0.0027	0.003	0.0029
	Hex.	0.0077	0.0029	0.0009	0.0027	0.0	-	-
$(Sc_{2/3}Nb_{1/3})_2C$	Rect	0.0126	0.0098	0.0073	0.0011	0.0061	0.0016	0.0
	Hex.	0.0147	0.0097	0.0084	0.0019	0.0	-	-
$(Sc_{2/3}Ta_{1/3})_2C$	Rect.	0.0054	0.0034	0.0	0.0014	0.004	0.0027	0.0025
	Hex.	0.0065	0.0037	0.0	0.0019	0.0025	-	-
$(Sc_{2/3}V_{1/3})_2C$	Rect.	0.0072	0.0072	0.0	0.0021	0.0031	0.024	0.0015
	Hex.	0.0061	0.0012	0.0	0.0008	0.0005	-	-
$(Ta_{2/3}Fe_{1/3})_2C$	Rect.	0.0278	0.0041	0.0	0.0147	0.0058	0.0099	0.022
	Hex.	0.0286	0.0037	0.0	0.0103	0.0152	-	-
$(Ta_{2/3}Sc_{1/3})_2C$	Rect.	0.0014	0.0006	0.0	0.0009	0.0009	0.0009	0.0009
	Hex.	0.0024	0.0009	0.0	0.0013	0.0013	-	-
$(Ti_{2/3}Cr_{1/3})_2C$	Rect.	0.0028	0.0018	0.0	0.0028	0.0024	0.0028	0.0021
	Hex.	0.0029	0.0019	0.0	0.0029	0.0028	-	-
$(Ti_{2/3}Mo_{1/3})_2C$	Rect.	0.0022	0.0003	0.0	0.0021	0.002	0.0021	0.0018
	Hex.	0.0029	0.0007	0.0	0.0025	0.0025	-	-
$(Ti_{2/3}Y_{1/3})_2C$	Rect.	0.0053	0.0014	0.0	0.0011	0.0013	0.0021	0.0027
	Hex.	0.0011	0.0009	0.0	0.0007	0.0009	-	-
$(V_{2/3}Sc_{1/3})_2C$	Rect.	0.0051	0.0036	0.0	0.0034	0.0033	0.0036	0.0033
	Hex.	0.0045	0.0043	0.0	0.0044	0.0041	-	-
$(V_{2/3}Ti_{1/3})_2C$	Rect.	0.0092	0.0029	0.0	0.0024	0.0026	0.0028	0.0027
	Hex.	0.0032	0.0013	0.0	0.0031	0.0026	-	-
$(Zr_{2/3}Hf_{1/3})_2C$	Rect.	0.0037	0.0036	0.0	0.0022	0.0016	0.0015	0.0008
	Hex.	0.0064	0.0051	0.0	0.0032	0.0036	-	-
$(Zr_{2/3}Mn_{1/3})_2C$	Rect.	0.0132	0.0106	0.0087	0.0016	0.0032	0.002	0.0
	Hex.	0.0126	0.0085	0.0075	0.0003	0.0	-	-
$(Zr_{2/3}Y_{1/3})_2C$	Rect.	0.0044	0.0019	0.0	0.0005	0.002	0.002	0.0009
	Hex.	0.0039	0.0019	0.0	0.0012	0.0008	-	-
$(Hf_{2/3}Fe_{1/3})_2N$	Rect.	0.0411	0.009	0.0088	0.0241	0.0139	0.0109	0.0
	Hex.	0.0413	0.0093	0.0085	0.0	0.0233	-	-
$(Hf_{2/3}Sc_{1/3})_2N$	Rect.	0.0104	0.0039	0.0007	0.0036	0.0006	0.0035	0.0
	Hex.	0.0041	0.0032	0.0	0.0031	0.0031	-	-
$(Ti_{2/3}Nb_{1/3})_2N$	Rect.	0.0025	0.002	0.0	0.0027	0.0024	0.0023	0.0024
	Hex.	0.0079	0.0022	0.0	0.0019	0.002	-	-
$(Ti_{2/3}V_{1/3})_2N$	Rect.	0.0027	0.0016	0.0	0.0025	0.0028	0.0026	0.0027
	Hex.	0.0029	0.0029	0.0	0.0029	0.0026	-	-
$(Zr_{2/3}Sc_{1/3})_2N$	Rect.	0.0179	0.0067	0.0	0.0124	0.0087	0.011	0.0073
	Hex.	0.0164	0.0076	0.0	0.0111	0.012	-	-

Table S5: Energy (in unit of eV/atom) compassion for i-MXene within various spin configurations in both rectangular (Rect.) and hexagonal (Hex.) lattice. (continued)

Compound	Structure	NM	FM	AFM-0	AFM-3 /AFM-β	AFM-2 /AFM-α	AFM-4	AFM-1
FM→ FM								
$(Zr_{2/3}Co_{1/3})_2N$	Rect.	0.0105	0.0011	0.0098	0.0099	0.0012	0.0	0.0012
	Hex.	0.0113	0.0012	0.0113	0.0	0.0105	-	-
$(Zr_{2/3}Mn_{1/3})_2N$	Rect.	0.0438	0.0114	0.0268	0.0	0.0151	0.0106	0.0162
	Hex.	0.0342	0.0002	0.0161	0.0	0.0041	-	-
$(Zr_{2/3}Y_{1/3})_2N$	Rect.	0.0041	0.0006	0.0146	0.0024	0.0024	0.0	0.0033
	Hex.	0.0039	0.0	0.0031	0.0026	0.0022	-	-
$(Zr_{2/3}Fe_{1/3})_2N$	Rect.	0.0451	0.011	0.0201	0.0264	0.0154	0.0	0.0177
	Hex.	0.0473	0.0094	0.0205	0.0	0.0278	-	-
$(Zr_{2/3}Hf_{1/3})_2N$	Rect.	0.0053	0.0	0.0119	0.0023	0.0031	0.0037	0.0014
	Hex.	0.0058	0.0	0.0052	0.004	0.0021	-	-
$(Hf_{2/3}Cr_{1/3})_2C$	Rect.	0.0034	0.0	0.0025	0.0036	0.0019	0.0017	0.0004
	Hex.	0.0034	0.0	0.0023	0.002	0.0034	-	-
$(Hf_{2/3}Hg_{1/3})_2C$	Rect.	0.0022	0.0	0.0007	0.0021	0.0012	0.0021	0.0012
	Hex.	0.0005	0.0	0.0002	0.0005	0.0005	-	-
$(Mo_{2/3}Cr_{1/3})_2C$	Rect.	0.0089	0.0004	0.0065	0.0	0.0017	0.0031	0.0021
	Hex.	0.0109	0.0	0.0068	0.0046	0.0006	-	-
$(Mo_{2/3}Fe_{1/3})_2C$	Rect.	0.0452	0.0	0.0021	0.0163	0.0087	0.0003	0.0083
	Hex.	0.0442	0.0002	0.0027	0.0	0.0158	-	-
$(Mo_{2/3}Mn_{1/3})_2C$	Rect.	0.0588	0.0	0.0077	0.021	0.0016	0.0021	0.0152
	Hex.	0.0594	0.0	0.008	0.0023	0.0214	-	-
$(Nb_{2/3}Co_{1/3})_2C$	Rect.	0.0039	0.0	0.0039	0.0037	0.0017	0.001	0.0017
	Hex.	0.0039	0.0	0.0039	0.0009	0.0036	-	-
$(Nb_{2/3}Fe_{1/3})_2C$	Rect.	0.0283	0.0	0.0024	0.012	0.0038	0.0059	0.0174
	Hex.	0.0288	0.0	0.0021	0.0061	0.0123	-	-
$(Ta_{2/3}Co_{1/3})_2C$	Rect.	0.0053	0.0	0.0053	0.0052	0.0031	0.0001	0.0016
	Hex.	0.0058	0.0	0.0058	0.0003	0.0059	-	-
$(Ta_{2/3}Mn_{1/3})_2C$	Rect.	0.0362	0.0079	0.0084	0.0053	0.0	0.0113	0.0146
	Hex.	0.0304	0.0021	0.0026	0.0	0.0055	-	-
$(Ti_{2/3}Nb_{1/3})_2C$	Rect.	0.0125	0.0	0.0012	0.0076	0.0051	0.0076	0.0038
	Hex.	0.0134	0.0	0.0017	0.0083	0.0083	-	-
$(Ti_{2/3}Pd_{1/3})_2C$	Rect.	0.0041	0.0	0.0041	0.0041	0.0013	0.0012	0.0013
	Hex.	0.0049	0.0	0.0049	0.0014	0.0049	-	-
$(Ti_{2/3}Sc_{1/3})_2C$	Rect.	0.0093	0.0	0.0007	0.0093	0.0093	0.0093	0.0093
	Hex.	0.0113	0.0	0.0016	0.0104	0.0104	-	-
$(Ti_{2/3}Ta_{1/3})_2C$	Rect.	0.0112	0.0	0.0003	0.0059	0.0055	0.0061	0.004
	Hex.	0.0134	0.0	0.0018	0.0071	0.0077	-	-
$(Ti_{2/3}Ti_{1/3})_2C$	Rect.	0.0278	0.0	0.0116	0.011	0.013	0.0087	0.0091
	Hex.	0.0414	0.0	0.014	0.028	0.0263	-	-
$(V_{2/3}Co_{1/3})_2C$	Rect.	0.0064	0.0	0.0052	0.0064	0.003	0.0024	0.003
	Hex.	0.0073	0.0	0.0063	0.0027	0.0073	-	-
$(V_{2/3}Fe_{1/3})_2C$	Rect.	0.0331	0.0	0.0039	0.0136	0.007	0.0088	0.0168
	Hex.	0.0335	0.0	0.0042	0.0092	0.014	-	-
$(V_{2/3}Mn_{1/3})_2C$	Rect.	0.0314	0.0037	0.0073	0.0	0.0006	0.005	0.0042
	Hex.	0.031	0.0035	0.0068	0.0	0.0047	-	-
$(V_{2/3}Rh_{1/3})_2C$	Rect.	0.0009	0.0	0.0009	0.0009	0.0009	0.0009	0.0009
	Hex.	0.0005	0.0	0.0005	0.0005	0.0005	-	-
$(Zr_{2/3}Cr_{1/3})_2C$	Rect.	0.0043	0.0	0.0028	0.0039	0.0033	0.0023	0.0009
	Hex.	0.0034	0.0	0.0018	0.0014	0.003	-	-
$(Zr_{2/3}Fe_{1/3})_2C$	Rect.	0.0159	0.0049	0.0081	0.0035	0.0003	0.0	0.0074
	Hex.	0.0168	0.0039	0.0072	0.0	0.0041	-	-
$(Zr_{2/3}Ni_{1/3})_2C$	Rect.	0.0037	0.0004	0.0037	0.0035	0.0014	0.0	0.0014
	Hex.	0.0041	0.0009	0.0041	0.0	0.0042	-	-
$(Hf_{2/3}Co_{1/3})_2N$	Rect.	0.0051	0.0	0.0033	0.0052	0.0005	0.0013	0.0005
	Hex.	0.0059	0.0	0.0059	0.001	0.0058	-	-
$(Hf_{2/3}Cr_{1/3})_2N$	Rect.	0.0078	0.0066	0.0078	0.0	0.0035	0.0074	0.0017
	Hex.	0.008	0.0064	0.0078	0.0	0.0072	-	-
$(Hf_{2/3}Mn_{1/3})_2N$	Rect.	0.0382	0.0032	0.0291	0.0091	0.0	0.0064	0.0073
	Hex.	0.036	0.0	0.0271	0.0032	0.0055	-	-
$(Hf_{2/3}Zr_{1/3})_2N$	Rect.	0.0025	0.0	0.0035	0.0029	0.0041	0.0027	0.0015
	Hex.	0.0031	0.0	0.0068	0.0031	0.0031	-	-
$(Ti_{2/3}Fe_{1/3})_2N$	Rect.	0.0408	0.0023	0.0152	0.0219	0.011	0.0	0.0135
	Hex.	0.0405	0.0023	0.0153	0.0	0.0219	-	-
$(Ti_{2/3}Hf_{1/3})_2N$	Rect.	0.0035	0.0	0.0017	0.0016	0.0016	0.0018	0.0016
	Hex.	0.0043	0.0	0.0026	0.0028	0.0023	-	-
$(Ti_{2/3}Mn_{1/3})_2N$	Rect.	0.0416	0.0	0.0239	0.0087	0.0005	0.0103	0.007
	Hex.	0.0413	0.0	0.0242	0.0101	0.008	-	-
$(Ti_{2/3}Sc_{1/3})_2N$	Rect.	0.0121	0.0	0.0004	0.0091	0.0085	0.0085	0.0085
	Hex.	0.0121	0.0	0.0091	0.0085	0.0092	-	-
$(Ti_{2/3}Ti_{1/3})_2N$	Rect.	0.0003	0.0	0.0003	0.006	0.0098	0.006	0.006
	Hex.	0.0144	0.0	0.0032	0.01	0.0083	-	-
$(Ti_{2/3}Y_{1/3})_2N$	Rect.	0.002	0.0	0.0013	0.0012	0.0016	0.0015	0.0015
	Hex.	0.0016	0.0	0.0012	0.0014	0.0012	-	-

Table S6: The atomic magnetic moments for transition mental atoms M and M′ in i-MXene $(M_{2/3}M'_{1/3})_2X$ within both rectangular and hexagonal lattices. Rect. and Hex. represent the rectangular and hexagonal lattice, respectively. M_M, $M_{M'}$ and M_{tot} are the magnetic moment for M (in unit of μ_B) atom, M′ atom (in unit of μ_B) and total magnetic moment (in unit of μ_B/f.u.).

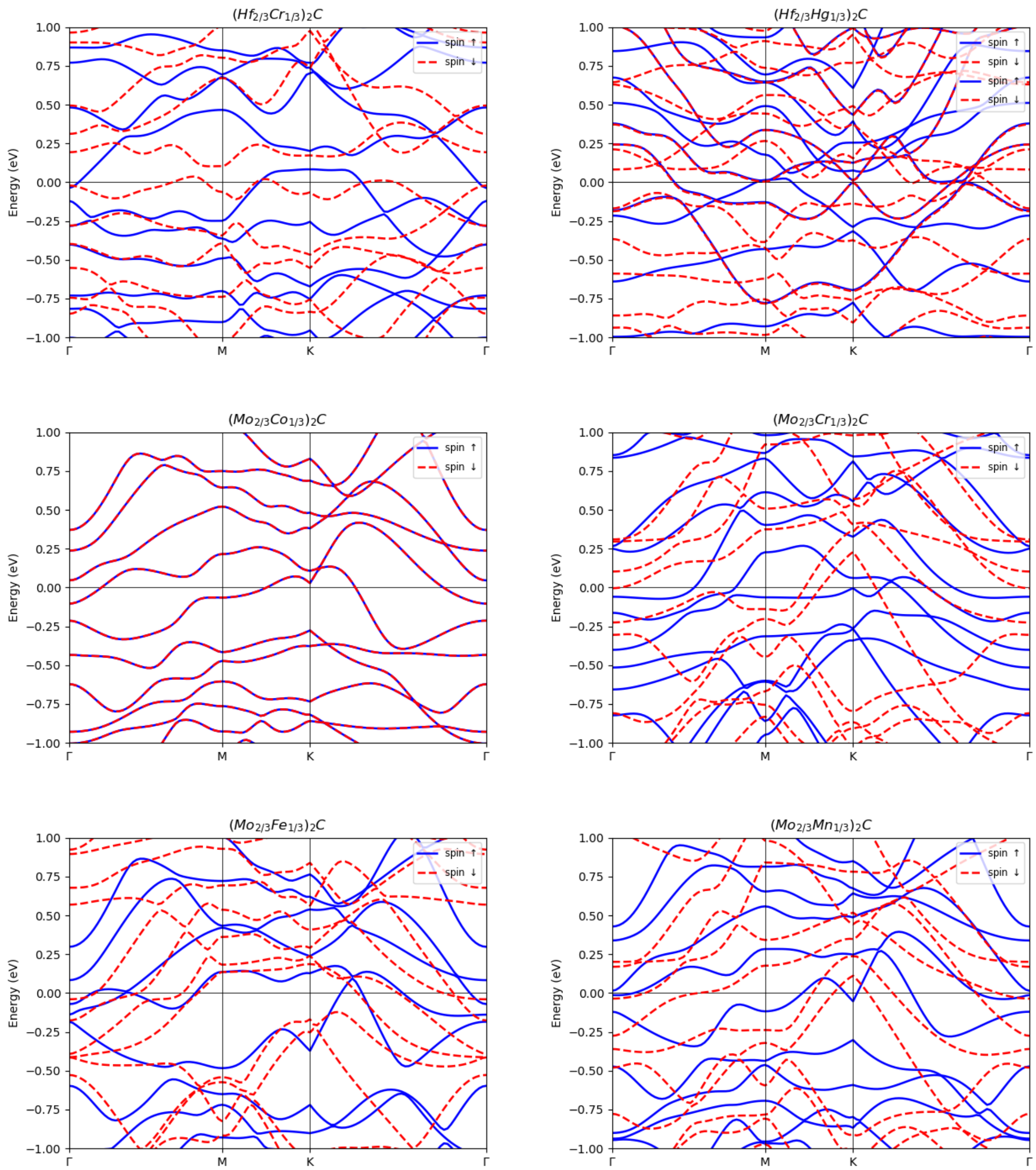
$(M_{2/3}M'_{1/3})_2X$	Rect.			Hex.		
	M_M	$M_{M'}$	M_{tot}	M_M	$M_{M'}$	M_{tot}
NM→FM						
$(Ti_{2/3}Ru_{1/3})_2C$	0	0	0	0.166	0.104	0.290
$(Zr_{2/3}Ti_{1/3})_2N$	0	0	0	0.470	0.54	0.950
$(Zr_{2/3}Cu_{1/3})_2C$	0	0	0	0.225	0.0	0.30
FM→FM						
$(Hf_{2/3}Cr_{1/3})_2C$	-0.014	0.664	0.412	-0.005	0.69	0.429
$(Hf_{2/3}Hg_{1/3})_2C$	0.185	0.021	0.257	0.258	0.031	0.344
$(Mo_{2/3}Cr_{1/3})_2C$	0.039	1.305	0.884	0.009	1.282	0.842
$(Mo_{2/3}Fe_{1/3})_2C$	-0.052	1.921	1.182	-0.046	1.905	1.173
$(Mo_{2/3}Mn_{1/3})_2C$	-0.111	2.235	1.295	-0.101	2.247	1.318
$(Nb_{2/3}Co_{1/3})_2C$	0.019	0.646	0.464	0.017	0.632	0.45
$(Nb_{2/3}Fe_{1/3})_2C$	-0.121	1.791	1.04	-0.099	1.794	1.047
$(Ta_{2/3}Co_{1/3})_2C$	-0.02	0.643	0.411	0.0	0.678	0.453
$(Ta_{2/3}Mn_{1/3})_2C$	-0.199	1.593	0.78	-0.2	1.581	0.771
$(Ti_{2/3}Nb_{1/3})_2C$	0.383	0.339	0.706	0.39	0.345	0.715
$(Ti_{2/3}Pd_{1/3})_2C$	0.281	0.037	0.377	0.287	0.037	0.382
$(Ti_{2/3}Sc_{1/3})_2C$	0.525	0.299	0.836	0.534	0.3	0.836
$(Ti_{2/3}Ta_{1/3})_2C$	0.359	0.405	0.725	0.354	0.392	0.718
$(Ti_{2/3}Ti_{1/3})_2C$	0.475	0.475	0.893	0.489	0.489	0.921
$(V_{2/3}Co_{1/3})_2C$	0.118	0.742	0.638	0.129	0.746	0.65
$(V_{2/3}Fe_{1/3})_2C$	-0.091	1.804	1.095	-0.059	1.814	1.127
$(V_{2/3}Mn_{1/3})_2C$	-0.261	1.575	0.697	-0.253	1.575	0.705
$(V_{2/3}Rh_{1/3})_2C$	0.217	0.051	0.303	0.13	0.031	0.303
$(Zr_{2/3}Cr_{1/3})_2C$	-0.033	0.665	0.383	-0.026	0.729	0.425
$(Zr_{2/3}Fe_{1/3})_2C$	-0.075	1.502	0.882	-0.047	1.515	0.917
$(Zr_{2/3}Ni_{1/3})_2C$	0.224	0.106	0.361	0.204	0.098	0.336
$(Hf_{2/3}Co_{1/3})_2N$	0.107	0.322	0.346	0.086	0.398	0.364
$(Hf_{2/3}Cr_{1/3})_2N$	0.091	-0.582	-0.267	-0.117	0.763	0.356
$(Hf_{2/3}Mn_{1/3})_2N$	-0.371	1.84	0.744	-0.391	1.791	0.686
$(Hf_{2/3}Zr_{1/3})_2N$	0.302	0.242	0.564	0.3	0.244	0.555
$(Ti_{2/3}Fe_{1/3})_2N$	-0.162	1.937	1.113	-0.166	1.932	1.102
$(Ti_{2/3}Hf_{1/3})_2N$	0.316	0.248	0.571	0.318	0.249	0.578
$(Ti_{2/3}Mn_{1/3})_2N$	-0.352	1.862	0.804	-0.355	1.869	0.809
$(Ti_{2/3}Sc_{1/3})_2N$	0.359	0.228	0.599	0.335	0.221	0.575
$(Ti_{2/3}Ti_{1/3})_2N$	0.306	0.52	0.579	0.301	0.301	0.575
$(Ti_{2/3}Y_{1/3})_2N$	0.237	0.142	0.397	0.219	0.135	0.378
$(Zr_{2/3}Co_{1/3})_2N$	0.034	-0.737	-0.459	0.029	-0.753	-0.469
$(Zr_{2/3}Fe_{1/3})_2N$	-0.063	1.959	1.235	-0.042	1.977	1.266
$(Zr_{2/3}Hf_{1/3})_2N$	0.254	0.295	0.526	0.251	0.296	0.53
$(Zr_{2/3}Mn_{1/3})_2N$	-0.088	1.782	1.064	-0.105	1.808	1.07
$(Zr_{2/3}Y_{1/3})_2N$	0.226	0.169	0.4	0.225	0.176	0.421

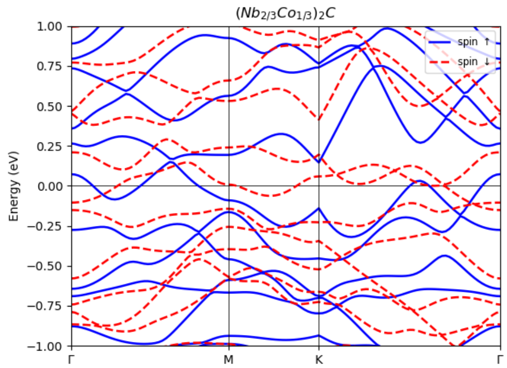
Table S7: The atomic magnetic moments for transition mental atoms M and M′ in i-MXene $(M_{2/3}M'_{1/3})_2X$ within both rectangular and hexagonal lattices. Rect. and Hex. represent the rectangular and hexagonal lattice, respectively. The magnetic moment is in unit of μ_B/atom. ↑ and ↓ denote the up and down layer transition atom, respectively.

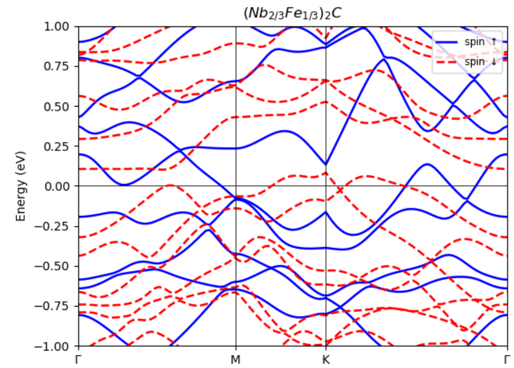
$(M_{2/3}M'_{1/3})_2X$	Rect.				Hex.			
	$M_{M\uparrow}$	$M_{M\downarrow}$	$M_{M'\uparrow}$	$M_{M'\downarrow}$	$M_{M\uparrow}$	$M_{M\downarrow}$	$M_{M'\uparrow}$	$M_{M'\downarrow}$
AFM→AFM								
$(Nb_{2/3}Mn_{1/3})_2C$	0.183	-0.183	1.555	-1.555	0.061	-0.061	1.807	-1.807
$(Nb_{2/3}Sc_{1/3})_2C$	0.251	-0.251	0.17	-0.17	0.263	-0.263	0.195	-0.195
$(Sc_{2/3}Cr_{1/3})_2C$	0.239	-0.239	1.241	-1.241	0.077	-0.077	1.409	-1.409
$(Sc_{2/3}Mn_{1/3})_2C$	0.145	-0.145	0.673	-0.673	0.028	-0.028	1.326	-1.326
$(Sc_{2/3}Mo_{1/3})_2C$	0.347	-0.347	0.624	-0.624	0.104	-0.104	0.449	-0.449
$(Sc_{2/3}Nb_{1/3})_2C$	0.205	-0.205	0.388	-0.388	0.185	-0.185	0.343	-0.343
$(Sc_{2/3}Ta_{1/3})_2C$	0.157	-0.157	0.357	-0.357	0.172	-0.172	0.349	-0.349
$(Sc_{2/3}V_{1/3})_2C$	0.298	-0.298	0.865	-0.865	0.148	-0.148	0.5	-0.5
$(Ta_{2/3}Fe_{1/3})_2C$	0.154	-0.154	1.816	-1.816	0.079	-0.079	1.723	-1.723
$(Ta_{2/3}Sc_{1/3})_2C$	0.297	-0.297	0.179	-0.179	0.269	-0.269	0.173	-0.173
$(Ti_{2/3}Cr_{1/3})_2C$	0.103	-0.103	0.166	-0.166	0.175	-0.175	0.438	-0.438
$(Ti_{2/3}Mo_{1/3})_2C$	0.132	-0.132	0.054	-0.054	0.181	-0.181	0.083	-0.083
$(Ti_{2/3}Y_{1/3})_2C$	0.46	-0.46	0.28	-0.28	0.202	-0.202	0.125	-0.125
$(V_{2/3}Sc_{1/3})_2C$	0.327	-0.327	0.119	-0.119	0.319	-0.319	0.126	-0.126
$(V_{2/3}Ti_{1/3})_2C$	0.282	-0.282	0.24	-0.24	0.335	-0.335	0.173	-0.173
$(Zr_{2/3}Hf_{1/3})_2C$	0.104	-0.104	0.134	-0.134	0.246	-0.246	0.289	-0.289
$(Zr_{2/3}Mn_{1/3})_2C$	0.016	-0.016	1.167	-1.167	0.117	-0.117	1.052	-1.052
$(Zr_{2/3}Y_{1/3})_2C$	0.183	-0.183	0.118	-0.118	0.221	-0.221	0.155	-0.155
$(Hf_{2/3}Fe_{1/3})_2N$	0.206	-0.206	1.936	-1.936	0.232	-0.232	1.934	-1.934
$(Hf_{2/3}Sc_{1/3})_2N$	0.236	-0.236	0.142	-0.142	0.319	-0.319	0.199	-0.199
$(Ti_{2/3}Nb_{1/3})_2N$	0.115	-0.115	0.156	-0.156	0.152	-0.152	0.246	-0.246
$(Ti_{2/3}V_{1/3})_2N$	0.129	-0.129	0.108	-0.108	0.167	-0.167	0.299	-0.299
$(Zr_{2/3}Sc_{1/3})_2N$	0.377	-0.377	0.3	-0.3	0.487	-0.487	0.357	-0.357
AFM→FM								
$(M_{2/3}M'_{1/3})_2X$	Rect.				Hex.			
	$M_{M\uparrow}$	$M_{M\downarrow}$	$M_{M'\uparrow}$	$M_{M'\downarrow}$	M_M	$M_{M'}$	M_{tot}	
$(Hf_{2/3}Fe_{1/3})_2C$	0.087	-0.087	1.04	-1.04	-0.137	1.623	0.899	
$(Hf_{2/3}Mn_{1/3})_2C$	0.128	-0.128	0.919	-0.919	-0.125	1.089	0.559	
$(Ti_{2/3}V_{1/3})_2C$	0.367	-0.367	0.698	-0.698	0.314	0.454	0.721	

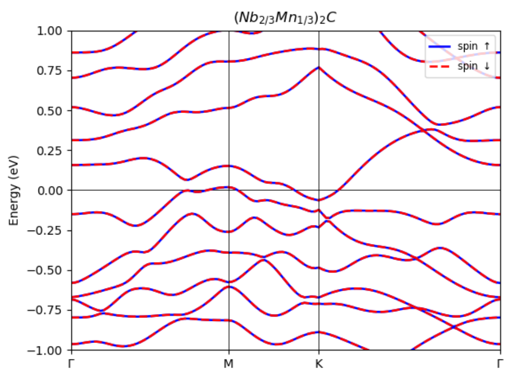
S9 band structures

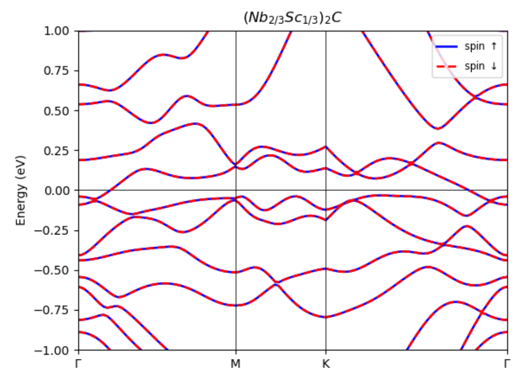
S9.1 magnetic i-MXene

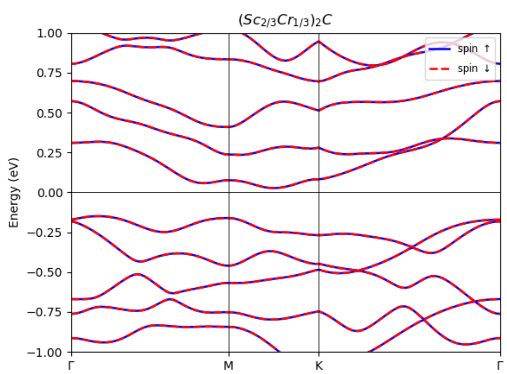


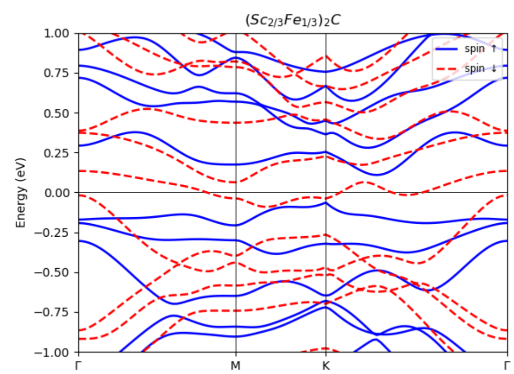

$(Nb_{2/3}Co_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

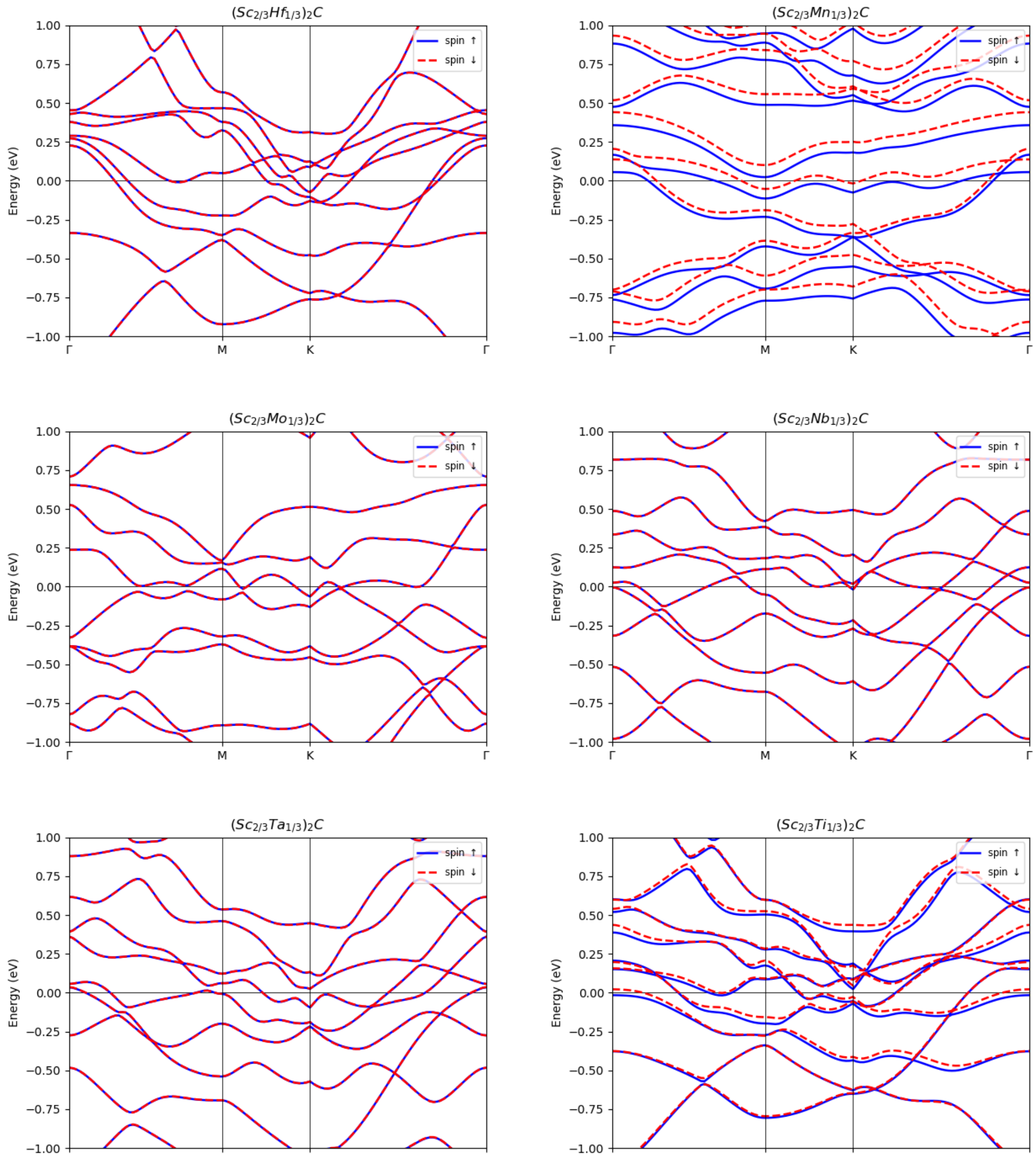

$(Nb_{2/3}Fe_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

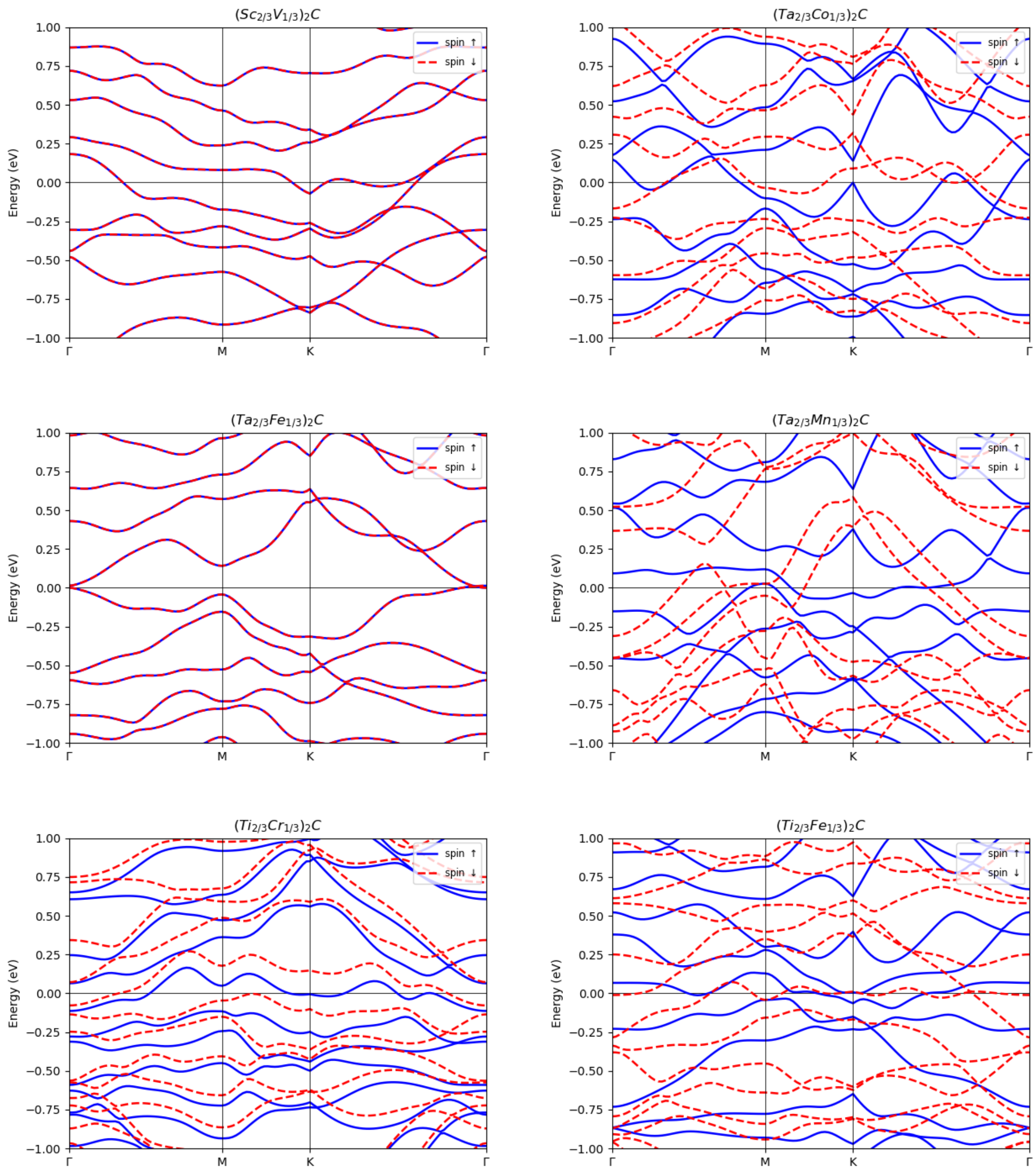

$(Nb_{2/3}Mn_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

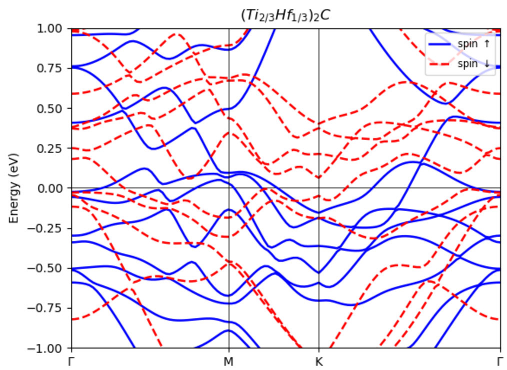

$(Nb_{2/3}Sc_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

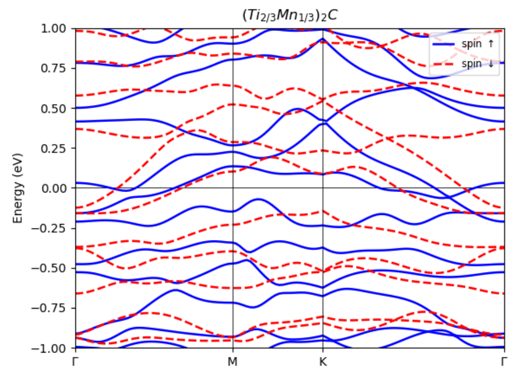

$(Sc_{2/3}Cr_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

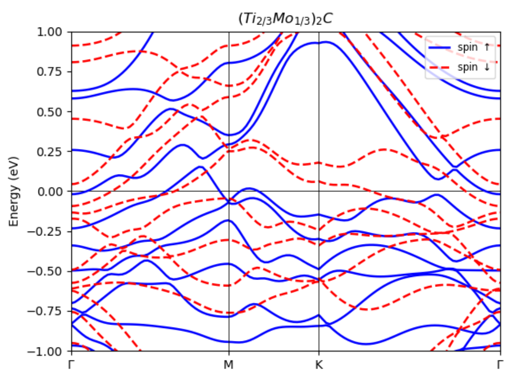

$(Sc_{2/3}Fe_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

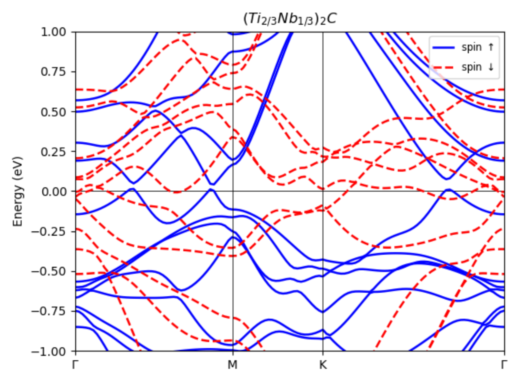

$(Sc_{2/3}Hf_{1/3})_2C$
$(Sc_{2/3}Mn_{1/3})_2C$
$(Sc_{2/3}Mo_{1/3})_2C$
$(Sc_{2/3}Nb_{1/3})_2C$
$(Sc_{2/3}Ta_{1/3})_2C$
$(Sc_{2/3}Ti_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ
M
K
Γ

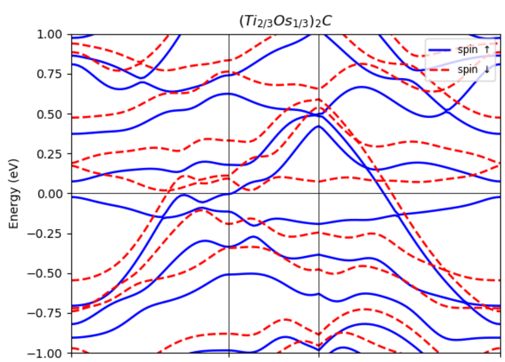

$(Sc_{2/3}V_{1/3})_2C$
$(Ta_{2/3}Co_{1/3})_2C$
$(Ta_{2/3}Fe_{1/3})_2C$
$(Ta_{2/3}Mn_{1/3})_2C$
$(Ti_{2/3}Cr_{1/3})_2C$
$(Ti_{2/3}Fe_{1/3})_2C$
Energy (eV)
Γ
M
K
spin ↑
spin ↓

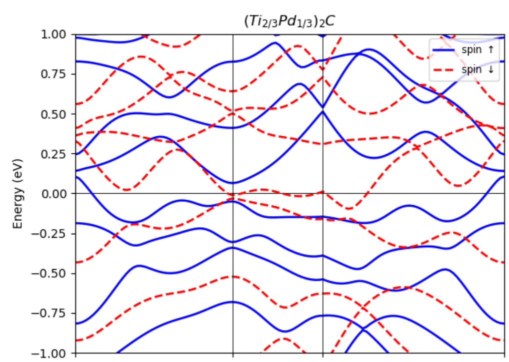

$(Ti_{2/3}Hf_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ

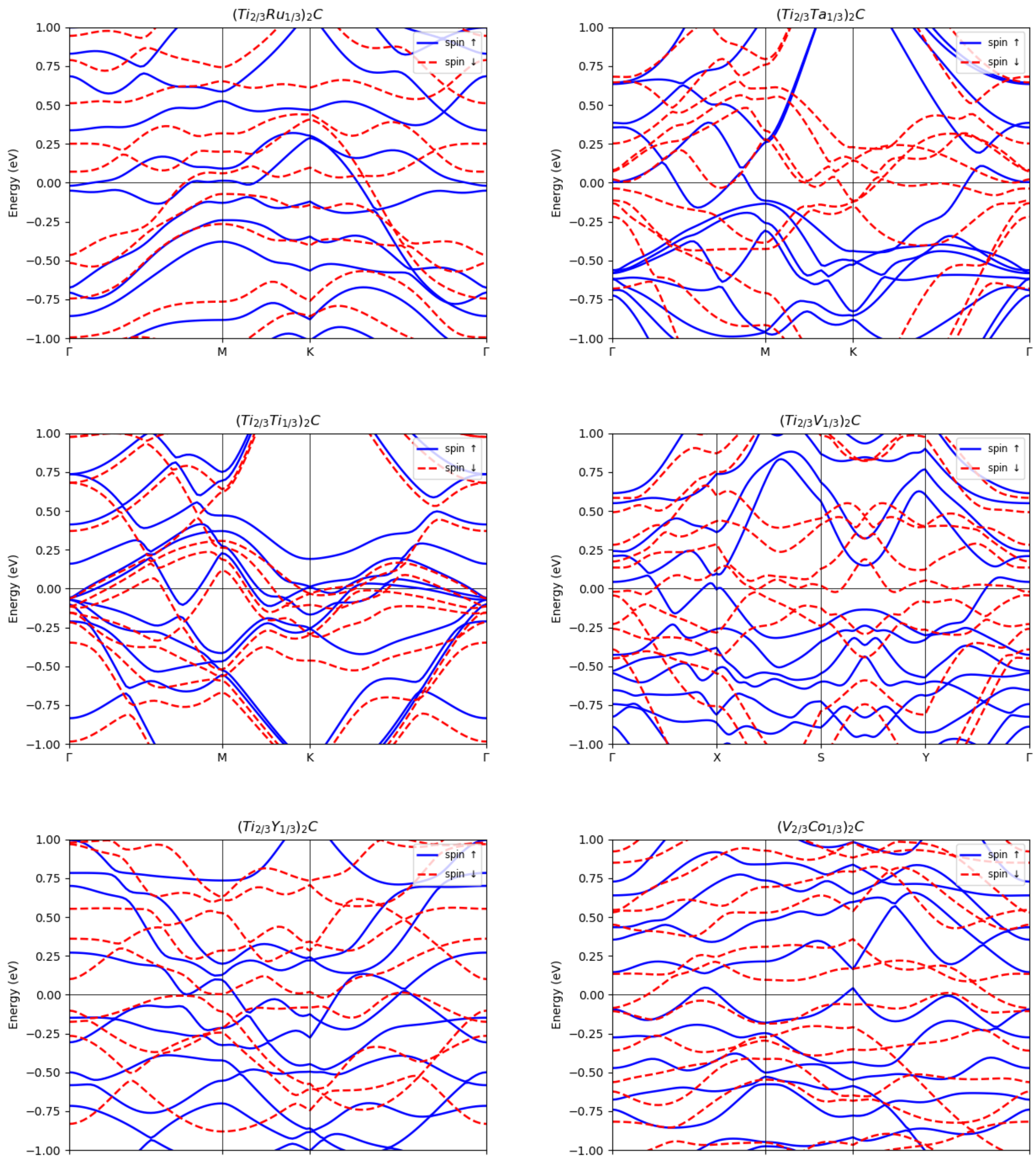

$(Ti_{2/3}Mn_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ


$(Ti_{2/3}Mo_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ

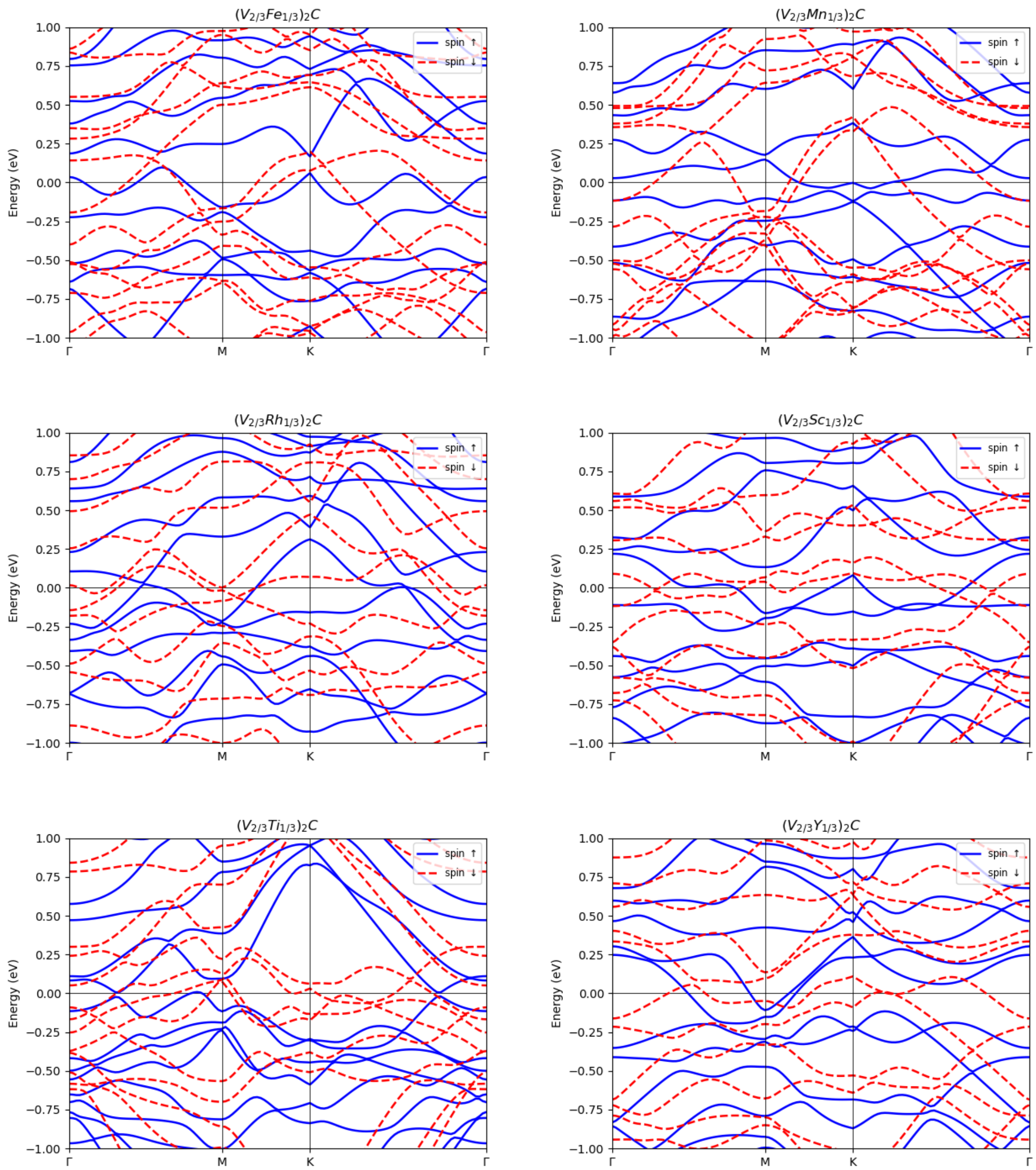

$(Ti_{2/3}Nb_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ


$(Ti_{2/3}Os_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ

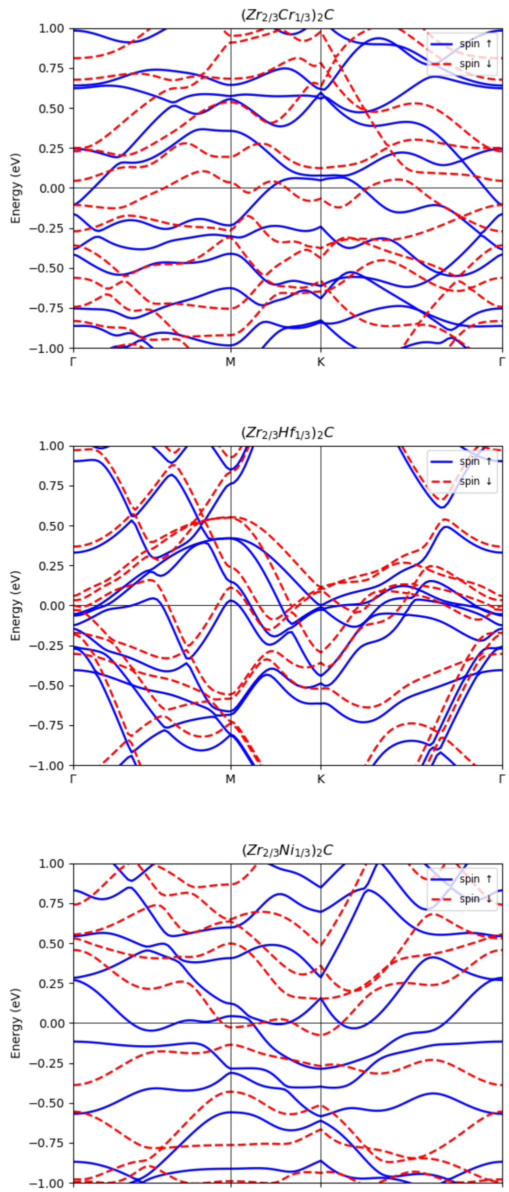

$(Ti_{2/3}Pd_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ M K Γ

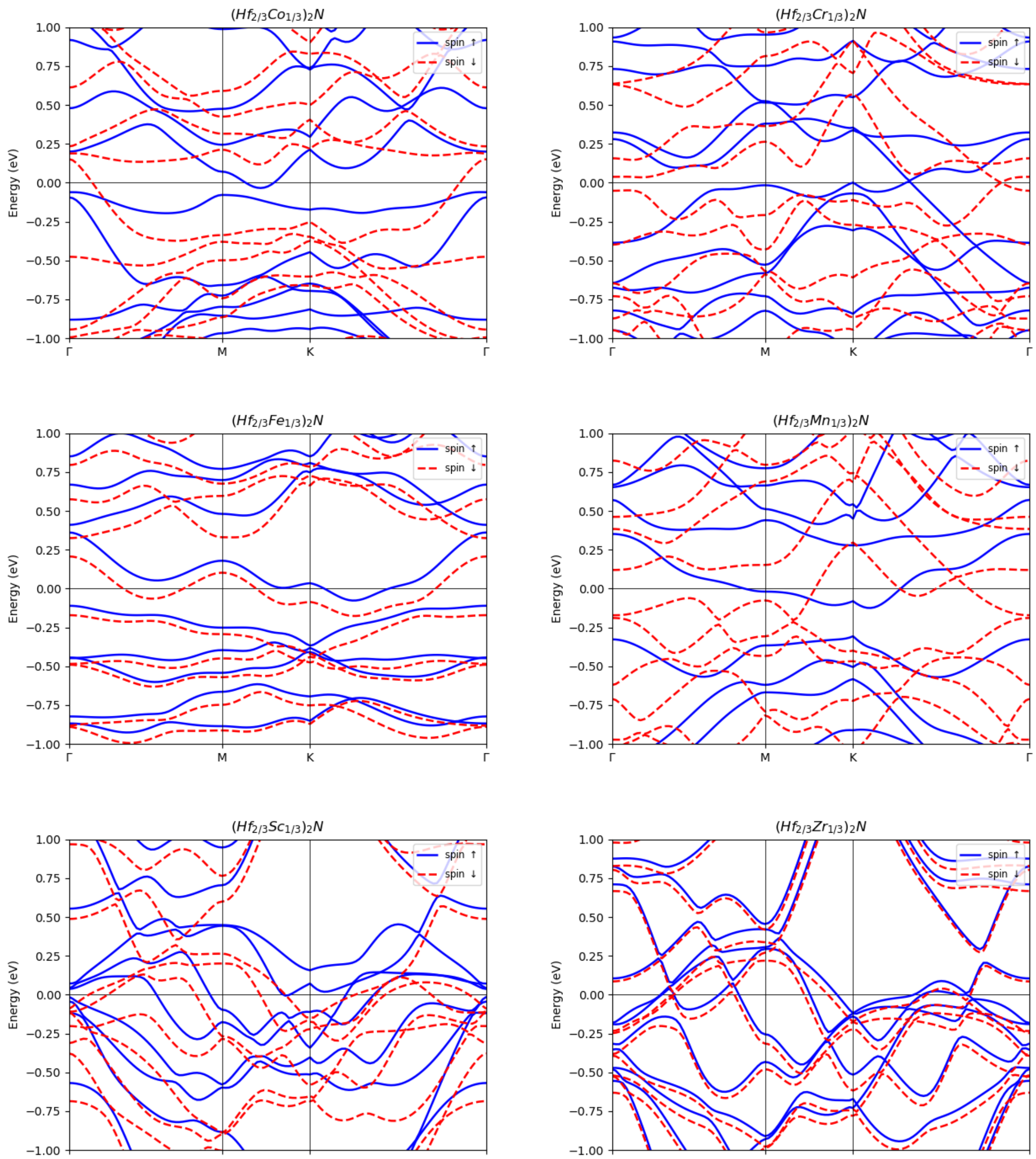


$(Ti_{2/3}Ru_{1/3})_2C$
$(Ti_{2/3}Ta_{1/3})_2C$
$(Ti_{2/3}Ti_{1/3})_2C$
$(Ti_{2/3}V_{1/3})_2C$
$(Ti_{2/3}Y_{1/3})_2C$
$(V_{2/3}Co_{1/3})_2C$
spin ↑
spin ↓
Energy (eV)
Γ M K Γ
Γ X S Y Γ



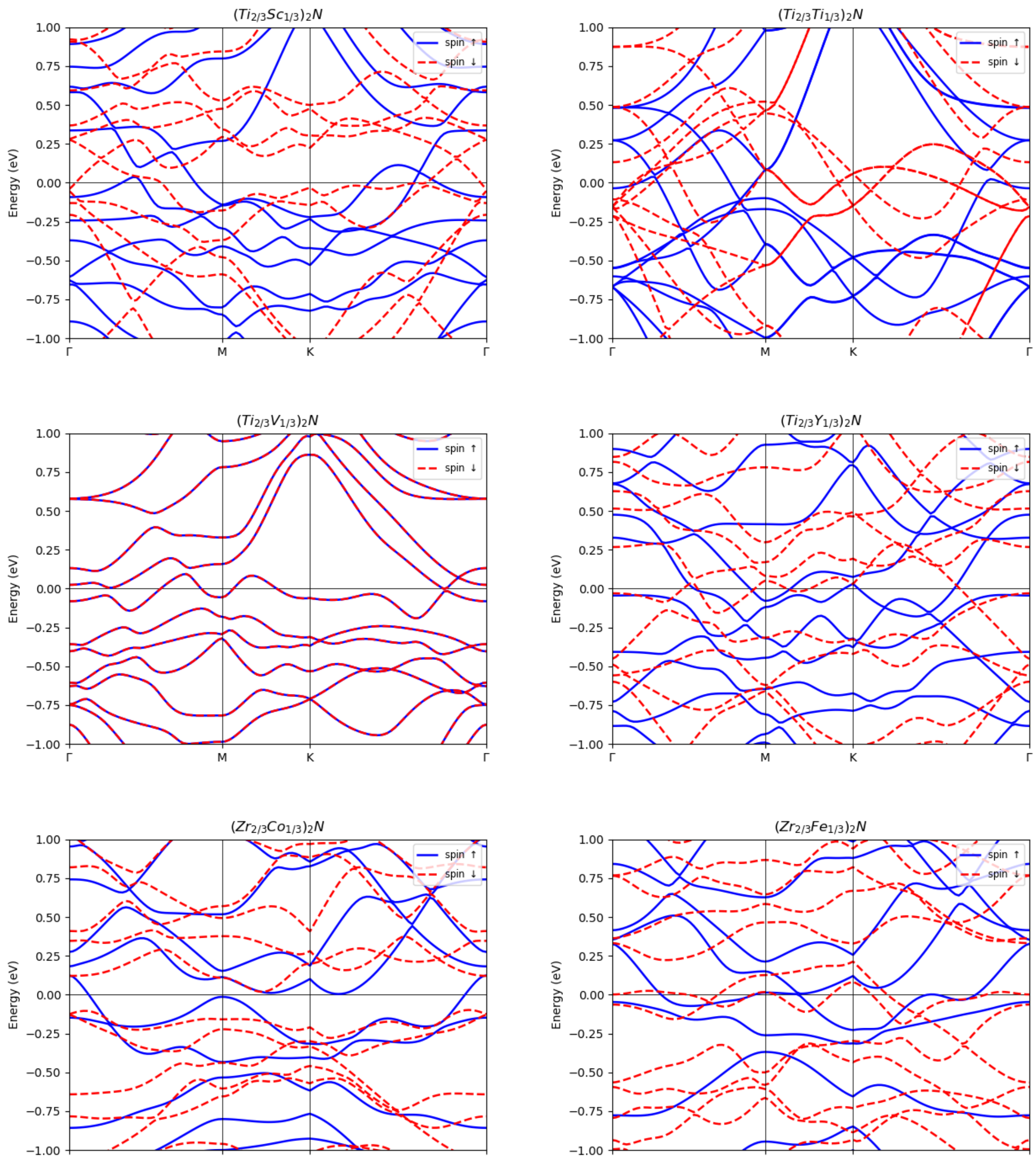
$(V_{2/3}Fe_{1/3})_2C$
$(V_{2/3}Mn_{1/3})_2C$
$(V_{2/3}Rh_{1/3})_2C$
$(V_{2/3}Sc_{1/3})_2C$
$(V_{2/3}Ti_{1/3})_2C$
$(V_{2/3}Y_{1/3})_2C$
spin ↑
spin ↓
Energy (eV)
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00


$(Zr_{2/3}Cr_{1/3})_2C$
$(Zr_{2/3}Fe_{1/3})_2C$
$(Zr_{2/3}Hf_{1/3})_2C$
$(Zr_{2/3}Mn_{1/3})_2C$
$(Zr_{2/3}Ni_{1/3})_2C$
$(Zr_{2/3}Y_{1/3})_2C$
Energy (eV)
spin ↑
spin ↓
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

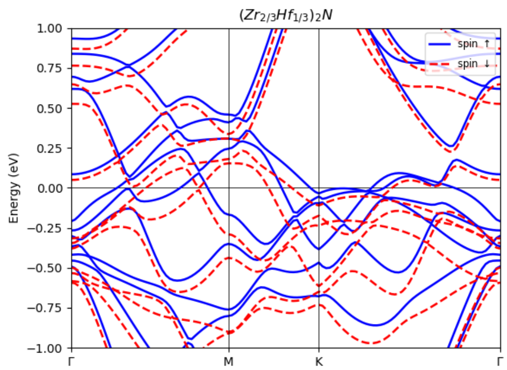


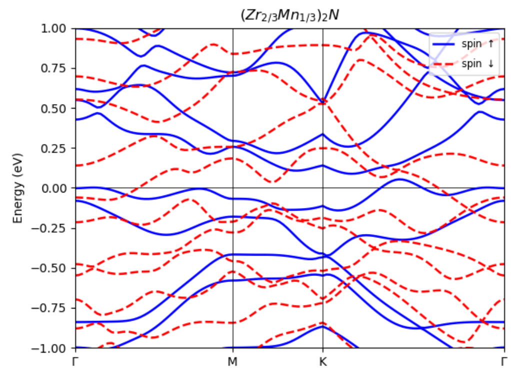
$(Hf_{2/3}Co_{1/3})_2N$
$(Hf_{2/3}Cr_{1/3})_2N$
$(Hf_{2/3}Fe_{1/3})_2N$
$(Hf_{2/3}Mn_{1/3})_2N$
$(Hf_{2/3}Sc_{1/3})_2N$
$(Hf_{2/3}Zr_{1/3})_2N$
spin ↑
spin ↓
Energy (eV)
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

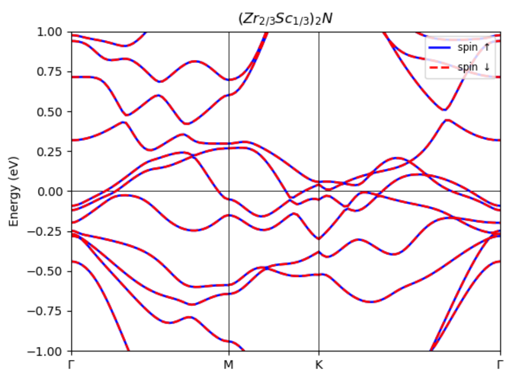

$(Ti_{2/3}Cd_{1/3})_2N$
$(Ti_{2/3}Fe_{1/3})_2N$
$(Ti_{2/3}Hf_{1/3})_2N$
$(Ti_{2/3}Hg_{1/3})_2N$
$(Ti_{2/3}Mn_{1/3})_2N$
$(Ti_{2/3}Nb_{1/3})_2N$
Energy (eV)
spin ↑
spin ↓
Γ
M
K
Γ

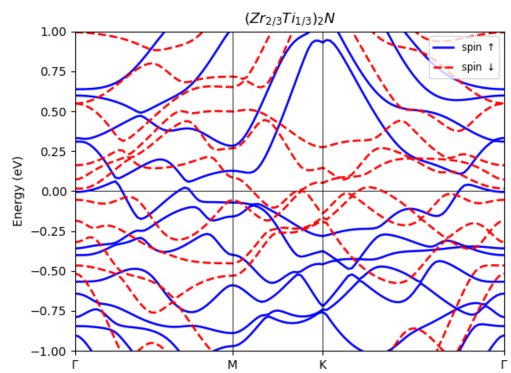


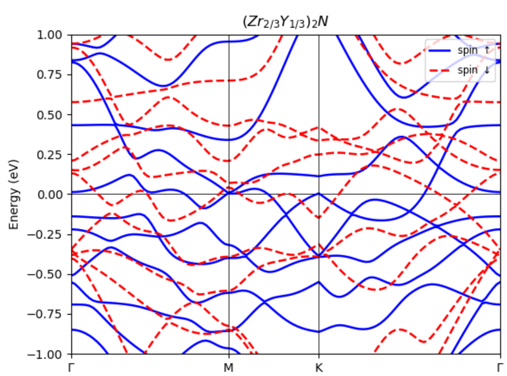
(Ti2/3Sc1/3)2N
(Ti2/3Ti1/3)2N
(Ti2/3V1/3)2N
(Ti2/3Y1/3)2N
(Zr2/3Co1/3)2N
(Zr2/3Fe1/3)2N
Energy (eV)
spin ↑
spin ↓
Γ
M
K
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00


$(Zr_{2/3}Hf_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

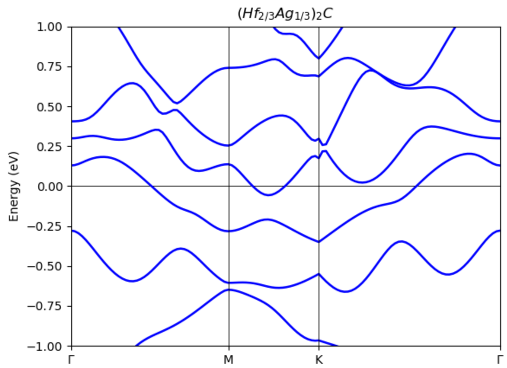

$(Zr_{2/3}Mn_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

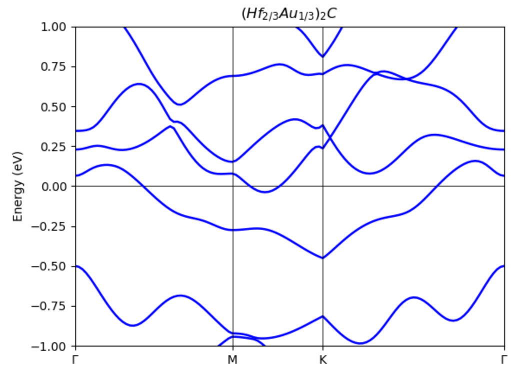

$(Zr_{2/3}Sc_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

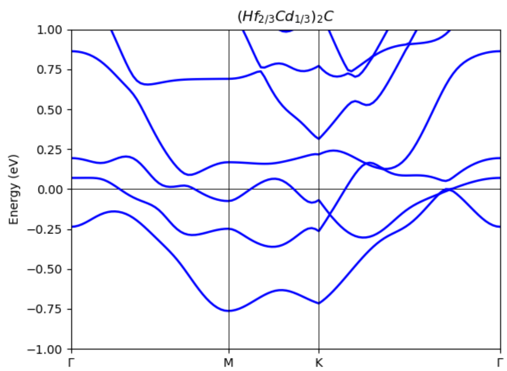

$(Zr_{2/3}Ti_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

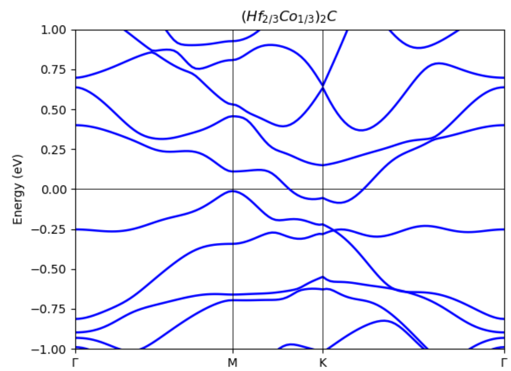

$(Zr_{2/3}Y_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
spin ↑
spin ↓

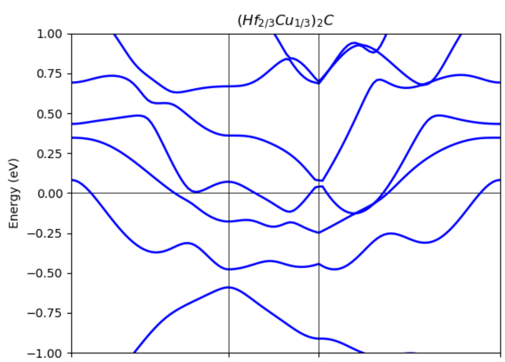
S9.2 Nonmagnetic i-MXene

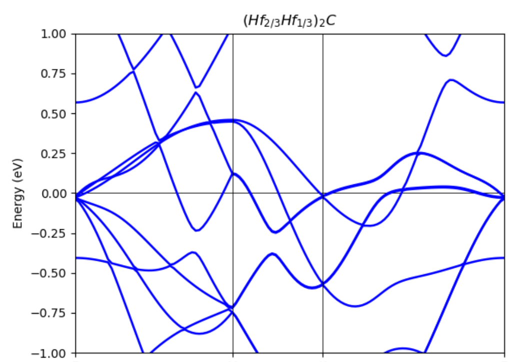


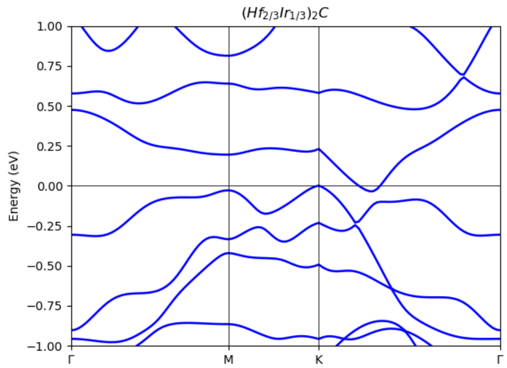


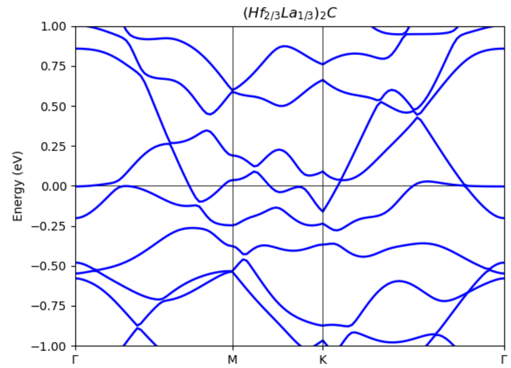


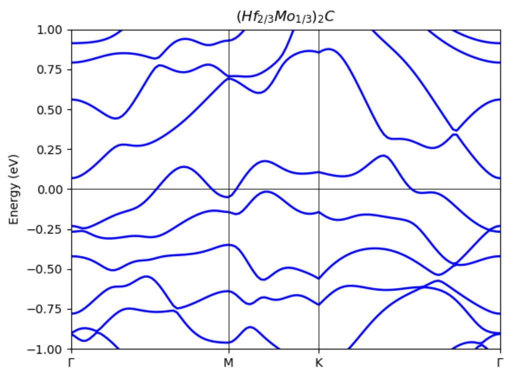


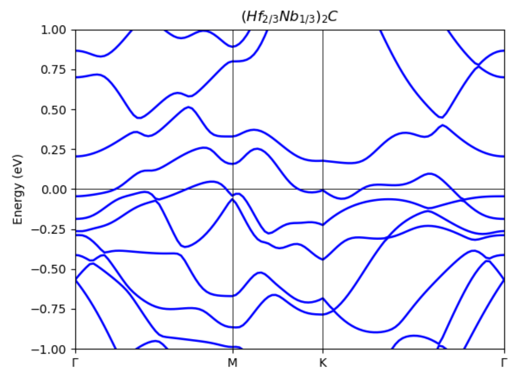


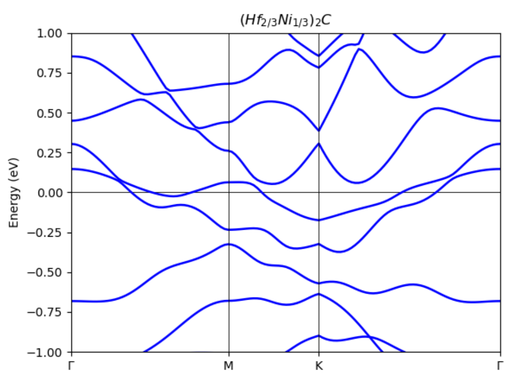


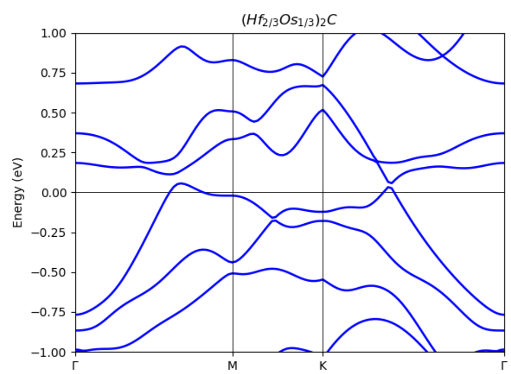

$(Hf_{2/3}Ir_{1/3})_2C$
Energy (eV)
Γ M K Γ

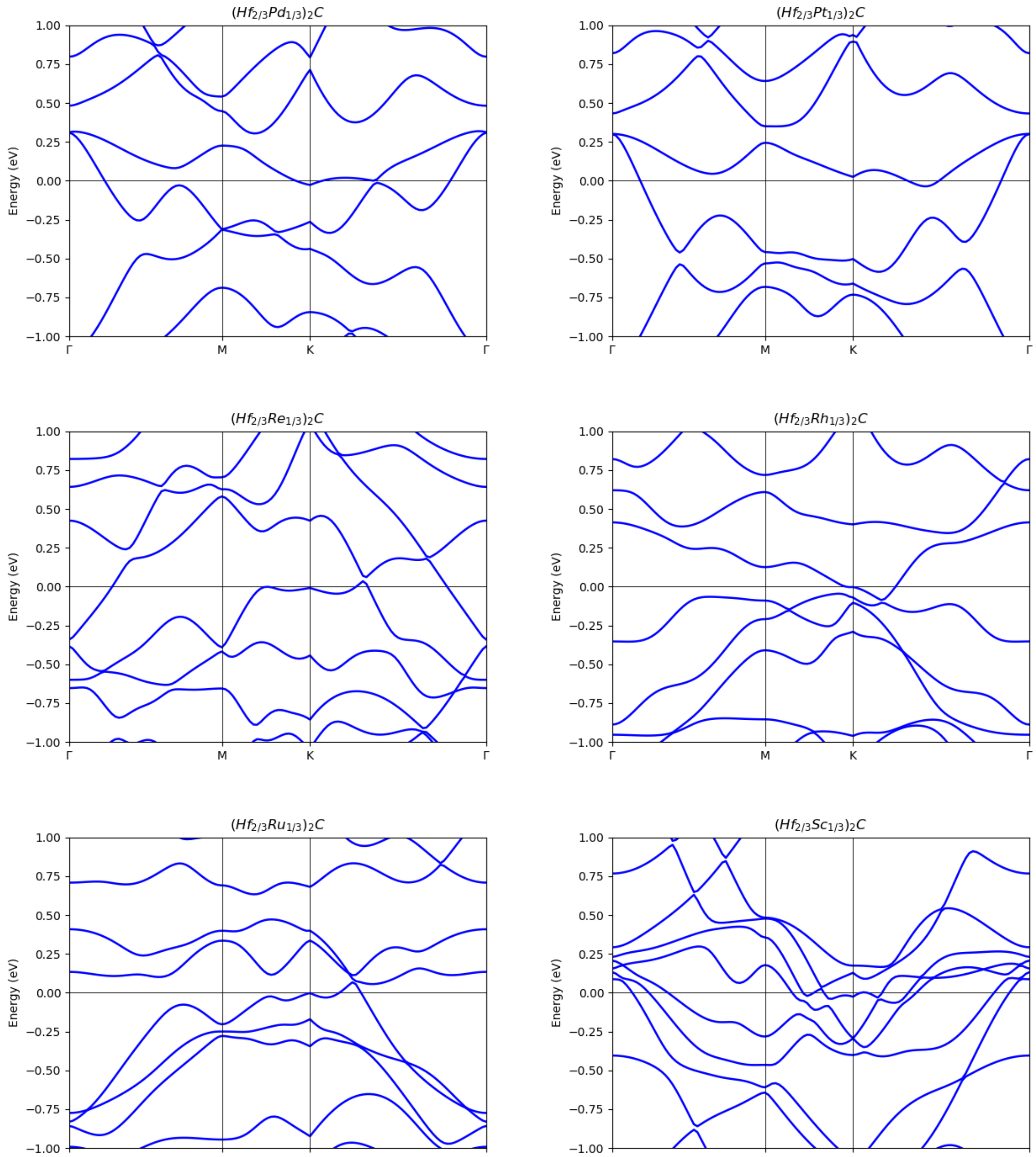

$(Hf_{2/3}La_{1/3})_2C$
Energy (eV)
Γ M K Γ

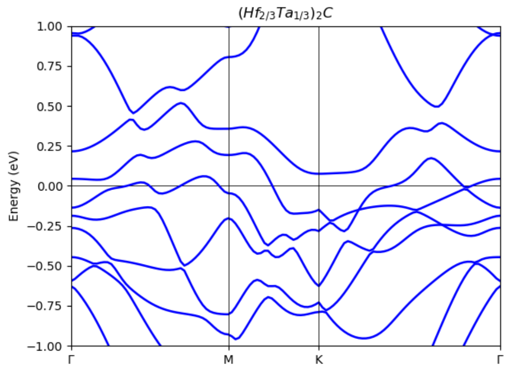

$(Hf_{2/3}Mo_{1/3})_2C$
Energy (eV)
Γ M K Γ

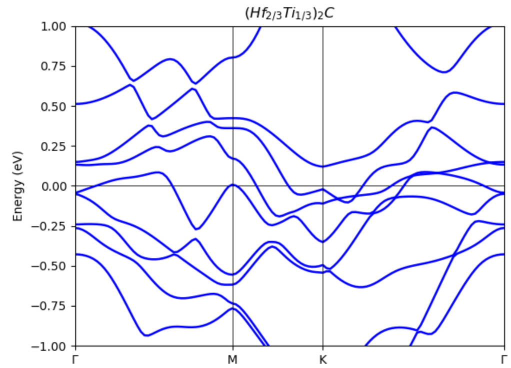

$(Hf_{2/3}Nb_{1/3})_2C$
Energy (eV)
Γ M K Γ

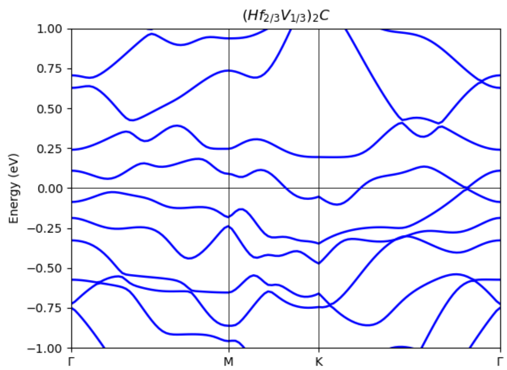

$(Hf_{2/3}Ni_{1/3})_2C$
Energy (eV)
Γ M K Γ

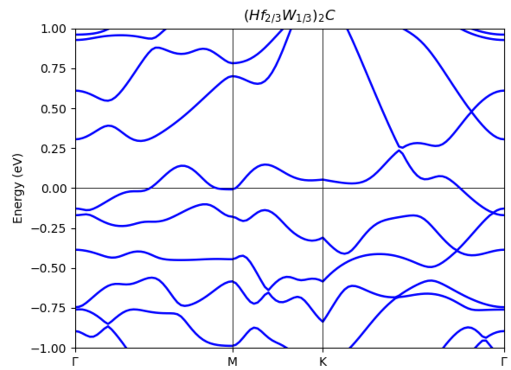

$(Hf_{2/3}Os_{1/3})_2C$
Energy (eV)
Γ M K Γ

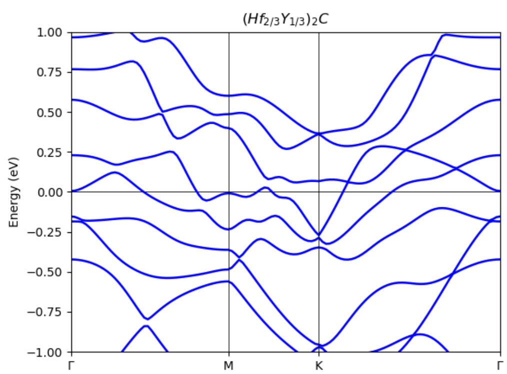

$(Hf_{2/3}Pd_{1/3})_2C$
$(Hf_{2/3}Pt_{1/3})_2C$
$(Hf_{2/3}Re_{1/3})_2C$
$(Hf_{2/3}Rh_{1/3})_2C$
$(Hf_{2/3}Ru_{1/3})_2C$
$(Hf_{2/3}Sc_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

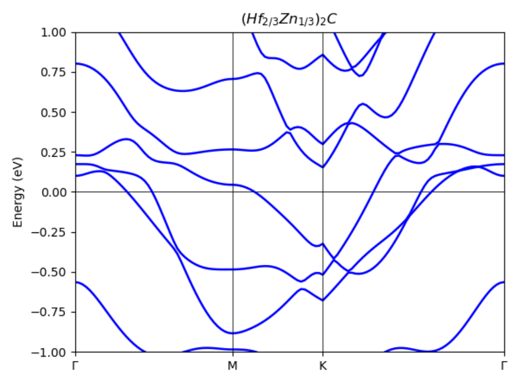

$(Hf_{2/3}Ta_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

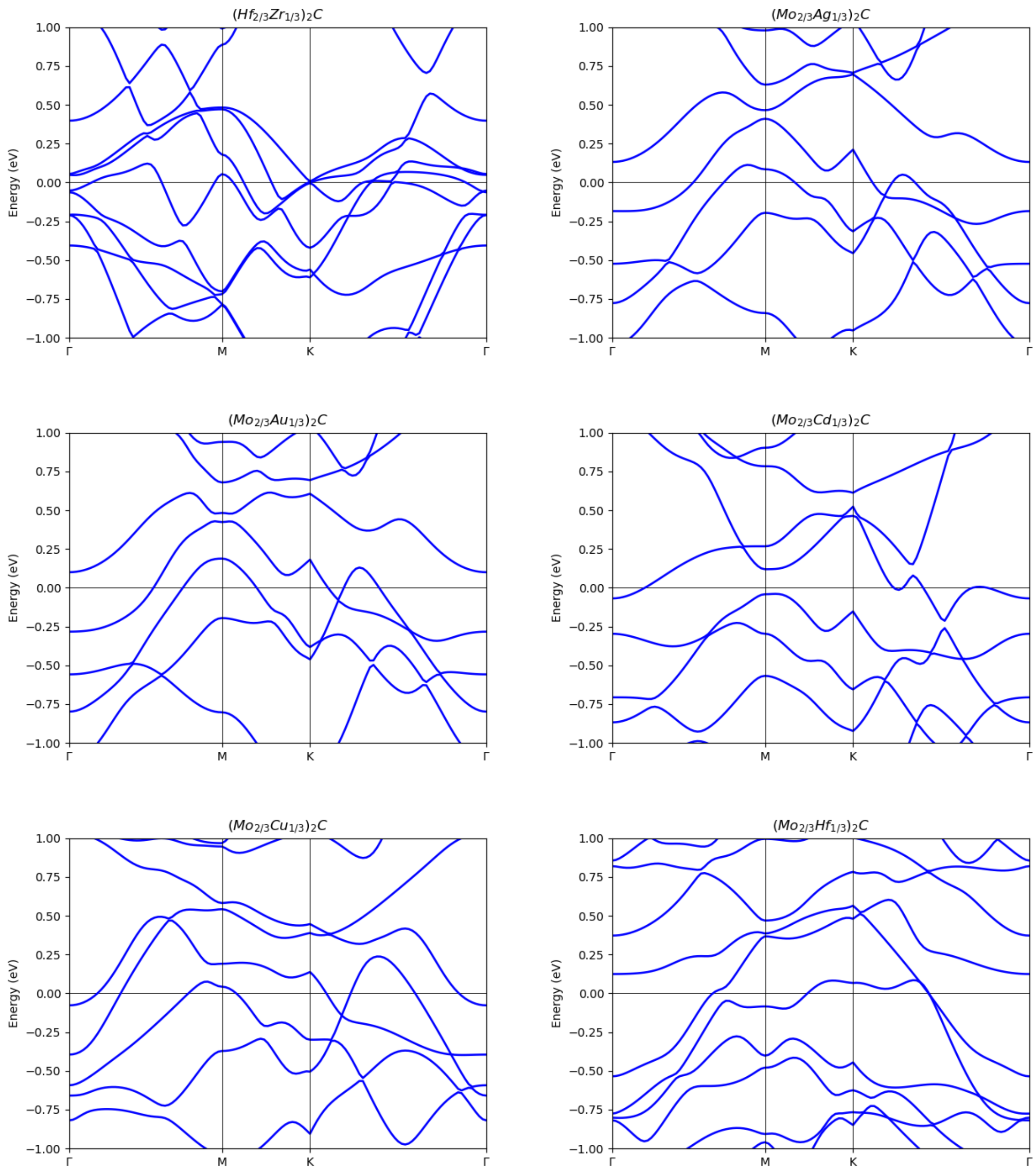

$(Hf_{2/3}Ti_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

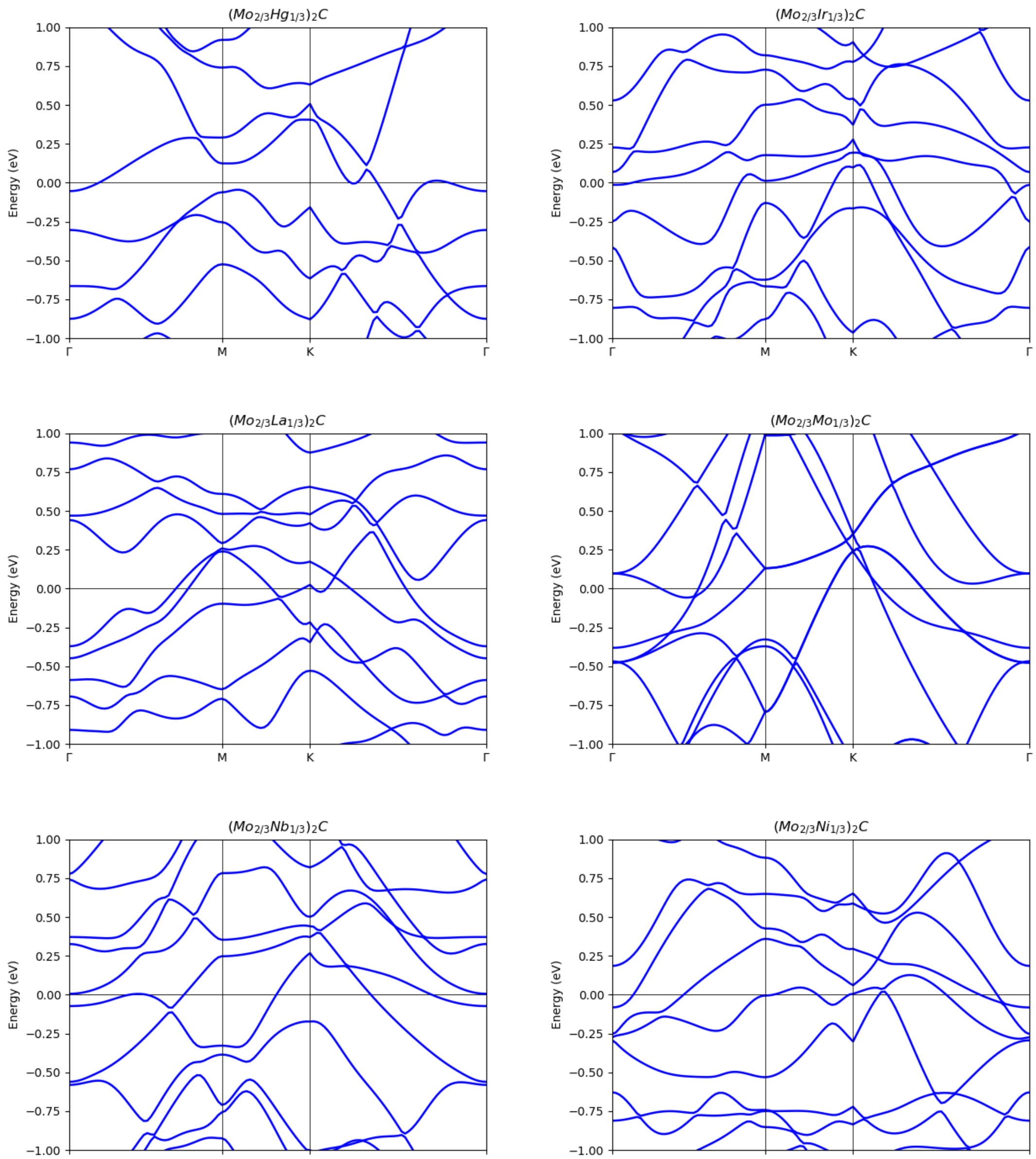

$(Hf_{2/3}V_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ


$(Hf_{2/3}W_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

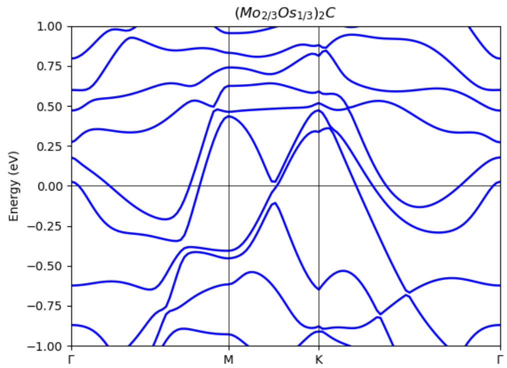

$(Hf_{2/3}Y_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

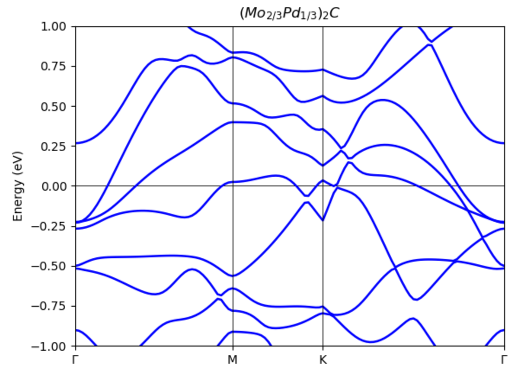

$(Hf_{2/3}Zn_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

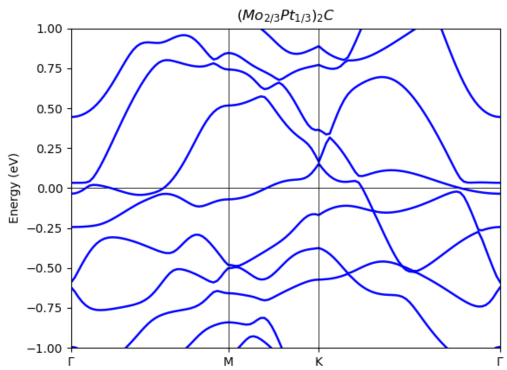

$(Hf_{2/3}Zr_{1/3})_2C$
$(Mo_{2/3}Ag_{1/3})_2C$
$(Mo_{2/3}Au_{1/3})_2C$
$(Mo_{2/3}Cd_{1/3})_2C$
$(Mo_{2/3}Cu_{1/3})_2C$
$(Mo_{2/3}Hf_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

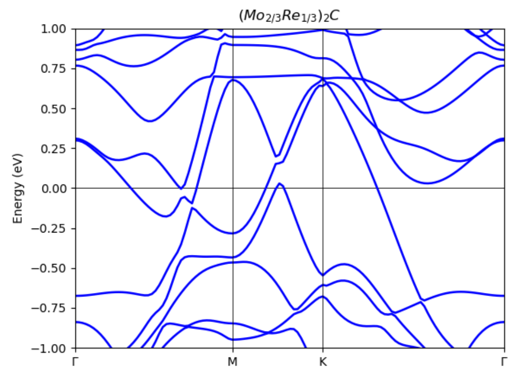


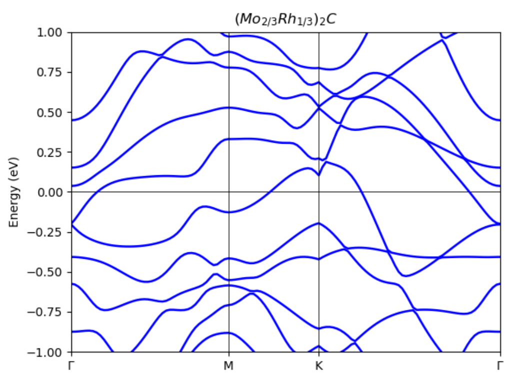
$(Mo_{2/3}Hg_{1/3})_2C$
$(Mo_{2/3}Ir_{1/3})_2C$
$(Mo_{2/3}La_{1/3})_2C$
$(Mo_{2/3}Mo_{1/3})_2C$
$(Mo_{2/3}Nb_{1/3})_2C$
$(Mo_{2/3}Ni_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

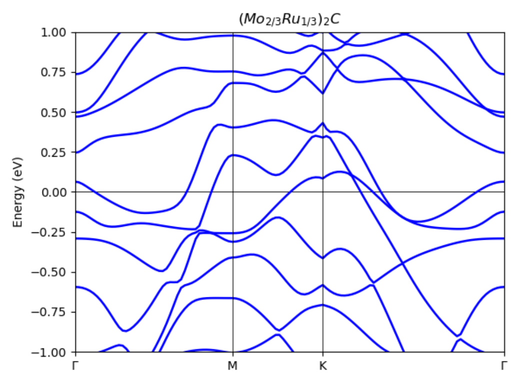

$(Mo_{2/3}Os_{1/3})_2C$
Energy (eV)
Γ M K Γ

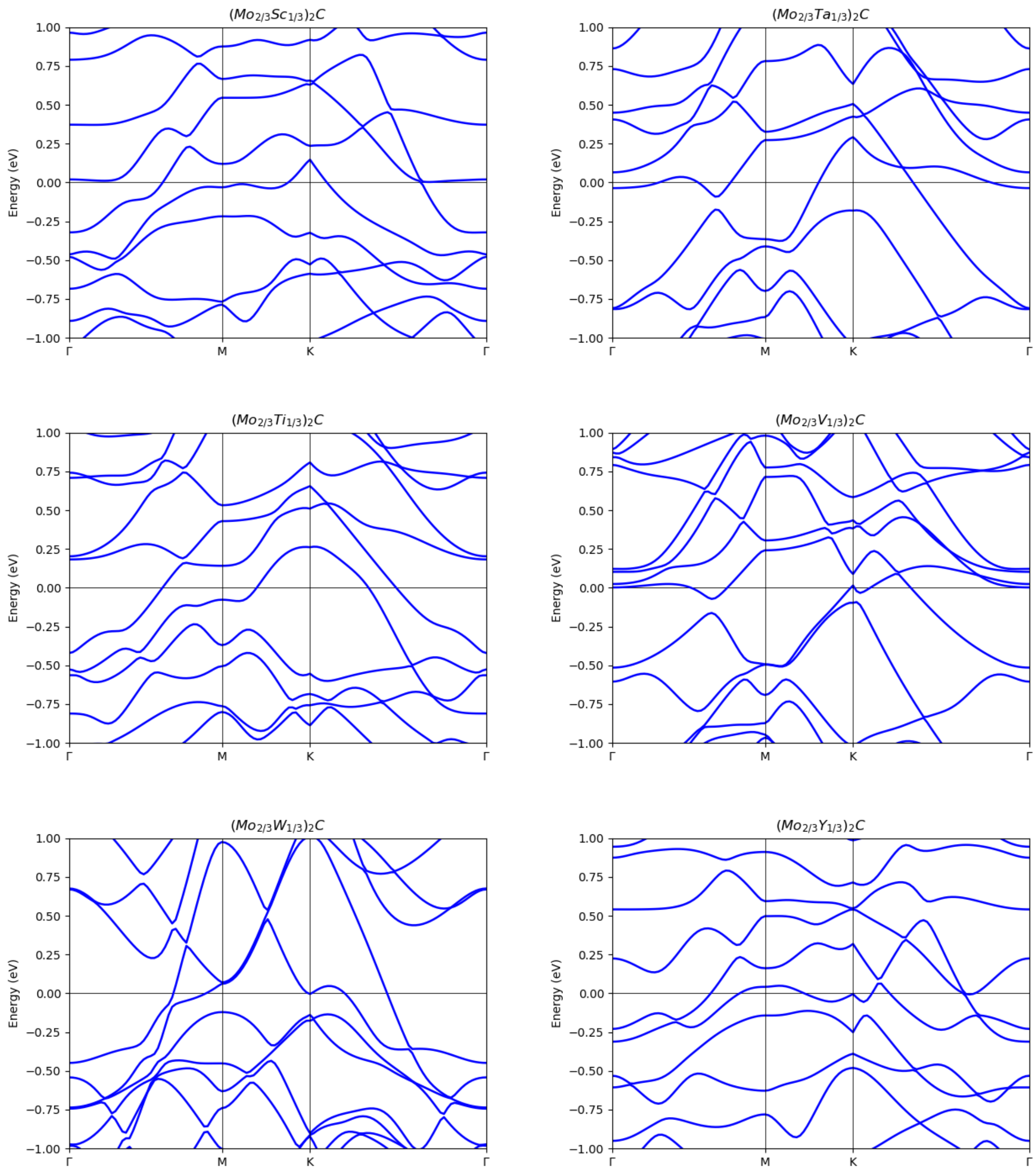

$(Mo_{2/3}Pd_{1/3})_2C$
Energy (eV)
Γ M K Γ

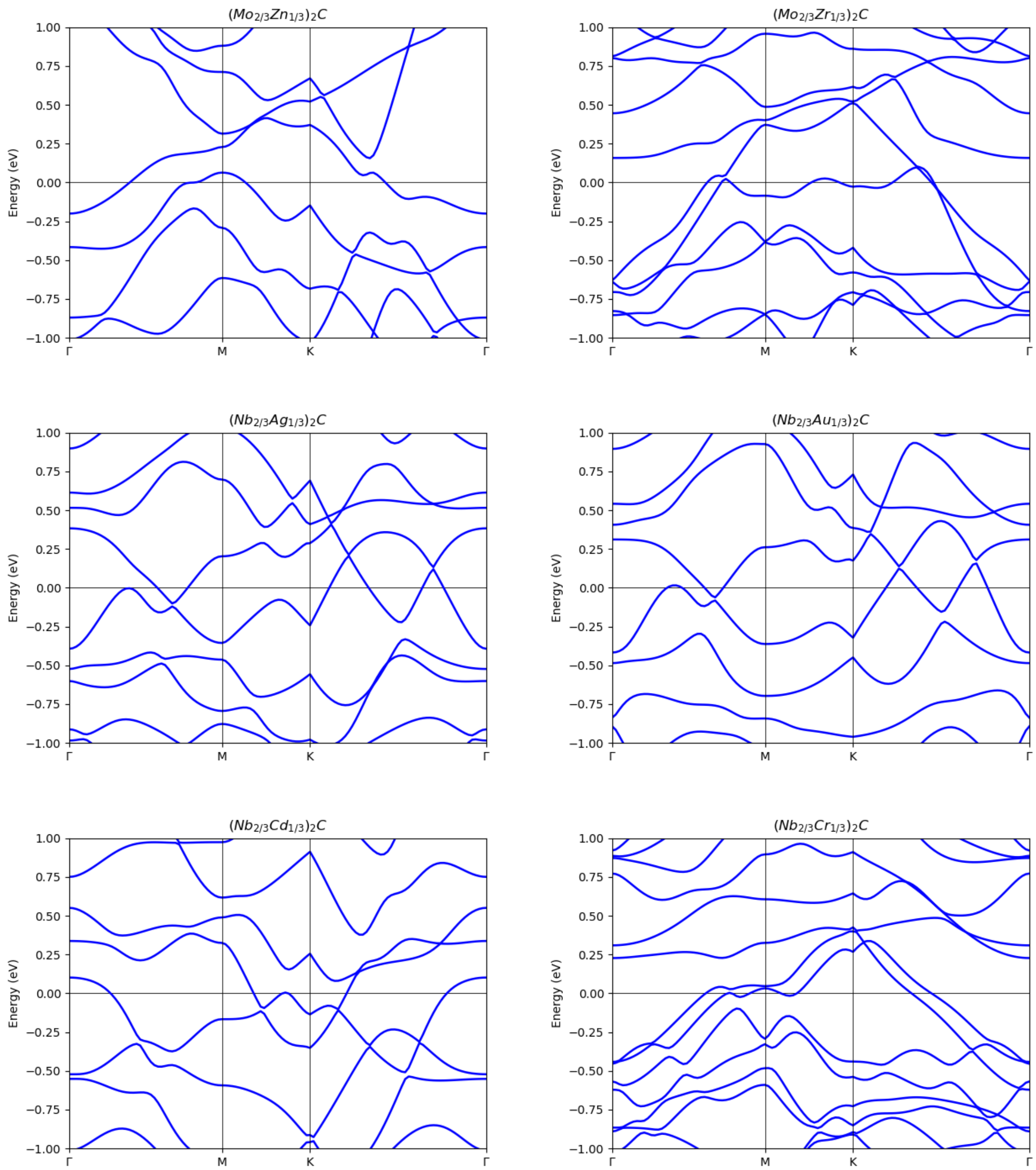

$(Mo_{2/3}Pt_{1/3})_2C$
Energy (eV)
Γ M K Γ


$(Mo_{2/3}Re_{1/3})_2C$
Energy (eV)
Γ M K Γ

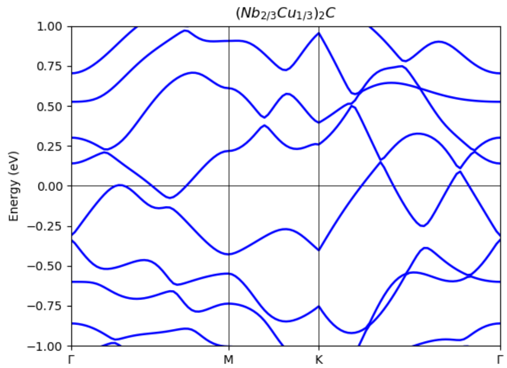

$(Mo_{2/3}Rh_{1/3})_2C$
Energy (eV)
Γ M K Γ

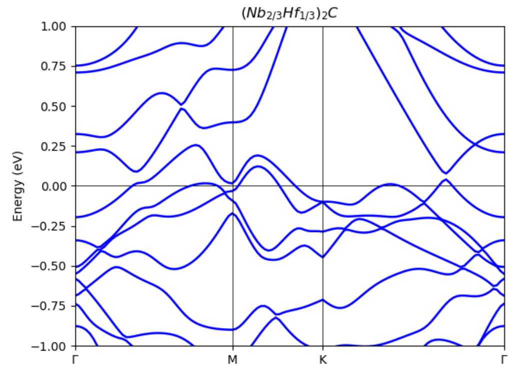

$(Mo_{2/3}Ru_{1/3})_2C$
Energy (eV)
Γ M K Γ

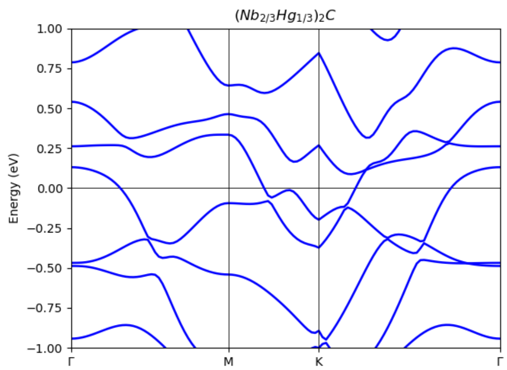

$(Mo_{2/3}Sc_{1/3})_2C$
$(Mo_{2/3}Ta_{1/3})_2C$
$(Mo_{2/3}Ti_{1/3})_2C$
$(Mo_{2/3}V_{1/3})_2C$
$(Mo_{2/3}W_{1/3})_2C$
$(Mo_{2/3}Y_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

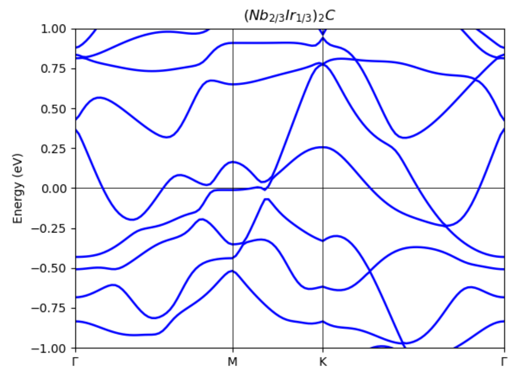


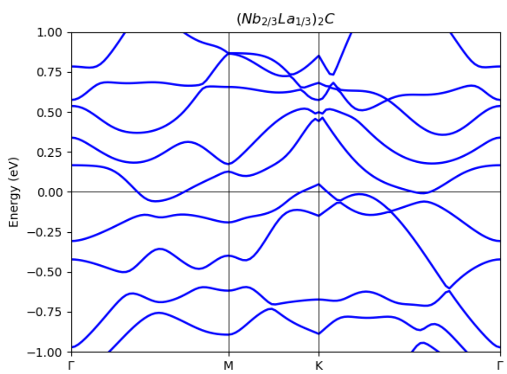
(Mo2/3Zn1/3)2C
(Mo2/3Zr1/3)2C
(Nb2/3Ag1/3)2C
(Nb2/3Au1/3)2C
(Nb2/3Cd1/3)2C
(Nb2/3Cr1/3)2C
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

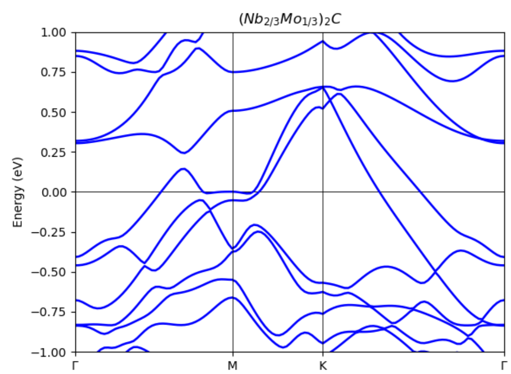

$(Nb_{2/3}Cu_{1/3})_2C$
Energy (eV)
Γ M K Γ

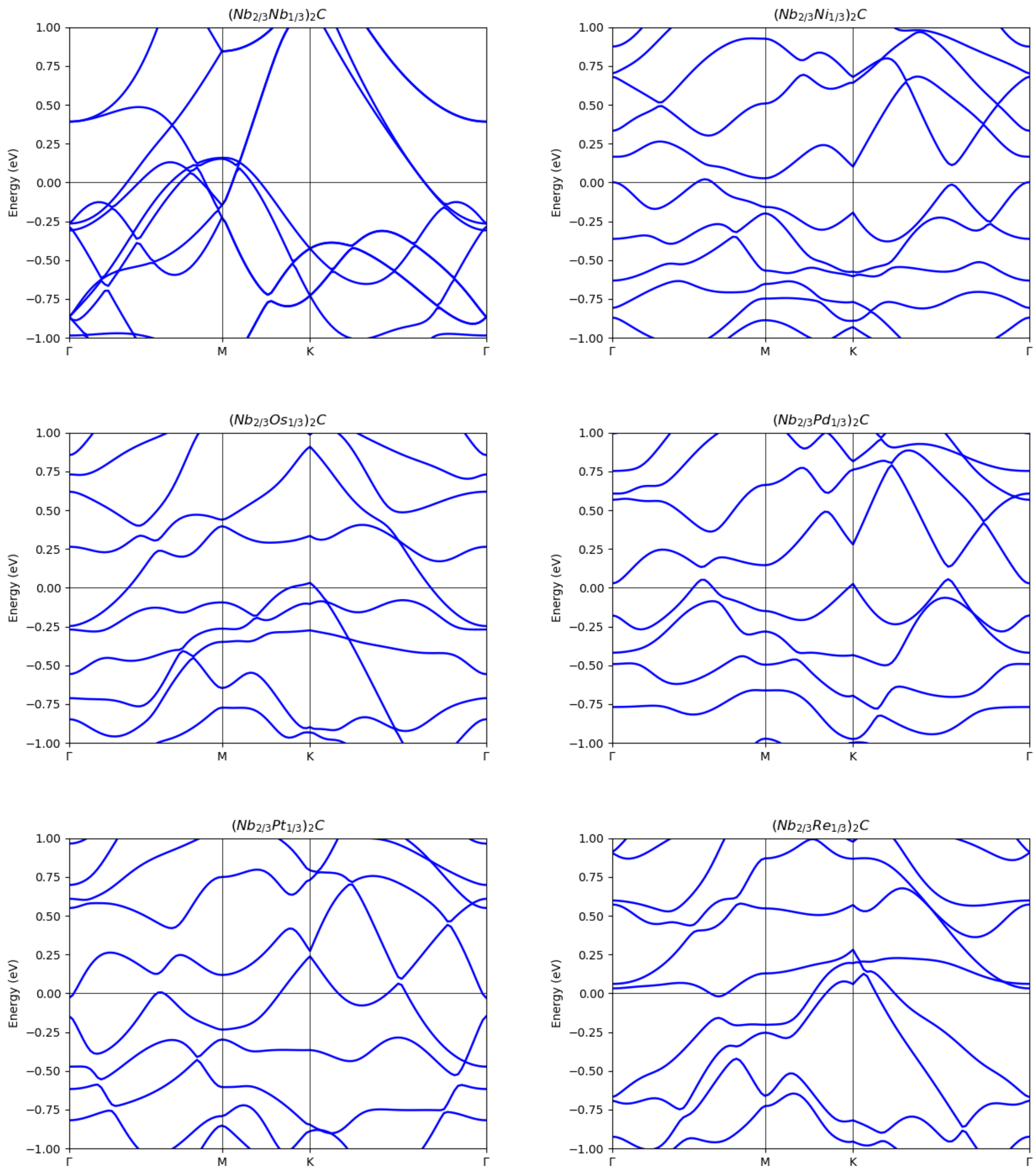

$(Nb_{2/3}Hf_{1/3})_2C$
Energy (eV)
Γ M K Γ

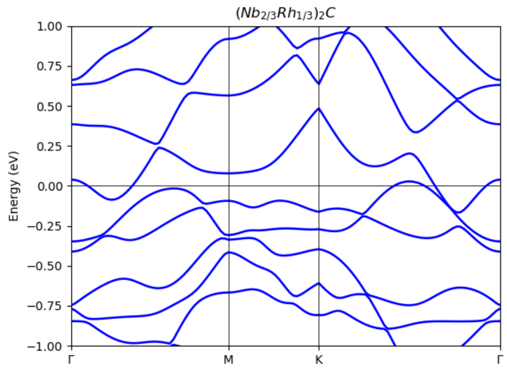

$(Nb_{2/3}Hg_{1/3})_2C$
Energy (eV)
Γ M K Γ

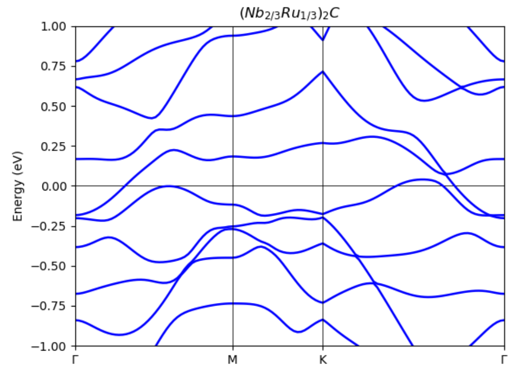

$(Nb_{2/3}Ir_{1/3})_2C$
Energy (eV)
Γ M K Γ

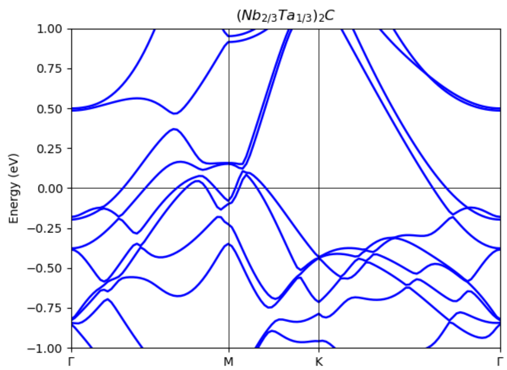

$(Nb_{2/3}La_{1/3})_2C$
Energy (eV)
Γ M K Γ

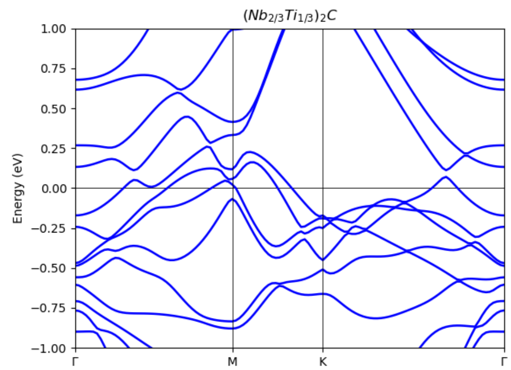

$(Nb_{2/3}Mo_{1/3})_2C$
Energy (eV)
Γ M K Γ

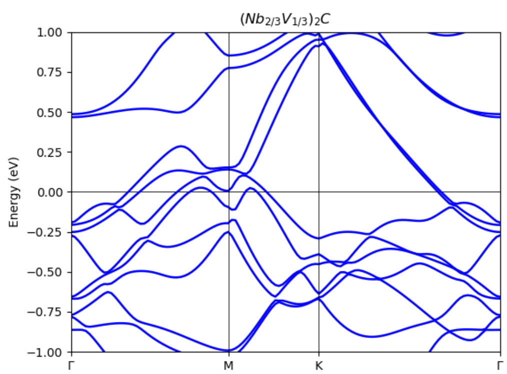

$(Nb_{2/3}Nb_{1/3})_2C$
$(Nb_{2/3}Ni_{1/3})_2C$
$(Nb_{2/3}Os_{1/3})_2C$
$(Nb_{2/3}Pd_{1/3})_2C$
$(Nb_{2/3}Pt_{1/3})_2C$
$(Nb_{2/3}Re_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

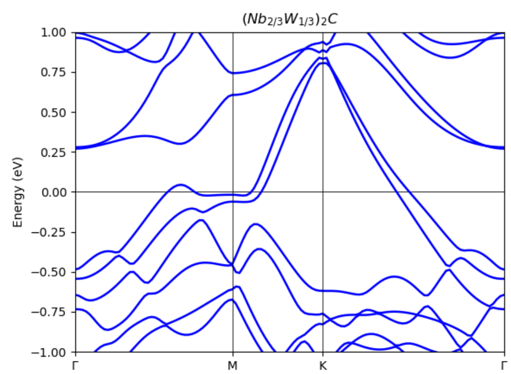

$(Nb_{2/3}Rh_{1/3})_2C$
Energy (eV)
Γ M K Γ

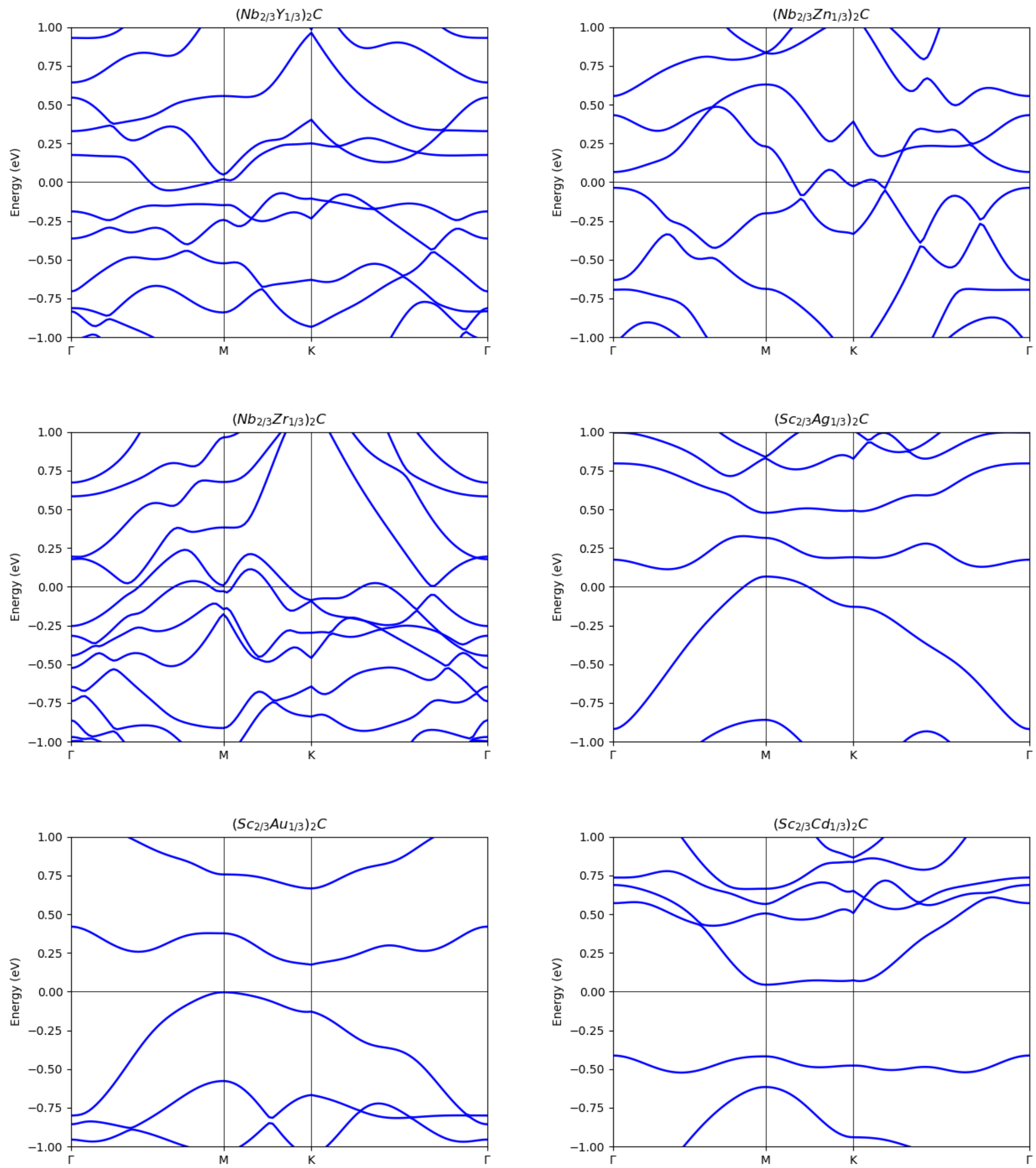

$(Nb_{2/3}Ru_{1/3})_2C$
Energy (eV)
Γ M K Γ


$(Nb_{2/3}Ta_{1/3})_2C$
Energy (eV)
Γ M K Γ


$(Nb_{2/3}Ti_{1/3})_2C$
Energy (eV)
Γ M K Γ

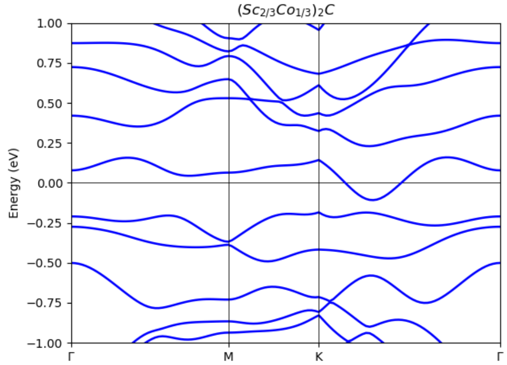

$(Nb_{2/3}V_{1/3})_2C$
Energy (eV)
Γ M K Γ


$(Nb_{2/3}W_{1/3})_2C$
Energy (eV)
Γ M K Γ

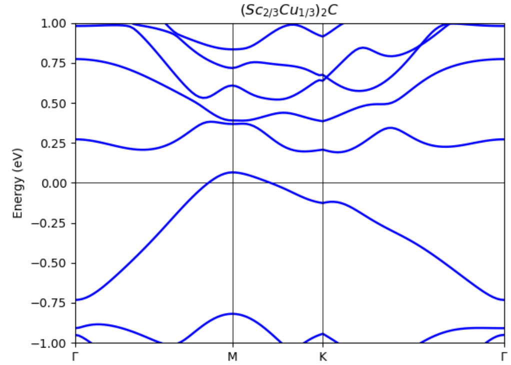


$(Nb_{2/3}Y_{1/3})_2C$
$(Nb_{2/3}Zn_{1/3})_2C$
$(Nb_{2/3}Zr_{1/3})_2C$
$(Sc_{2/3}Ag_{1/3})_2C$
$(Sc_{2/3}Au_{1/3})_2C$
$(Sc_{2/3}Cd_{1/3})_2C$
Energy (eV)
Γ
M
K

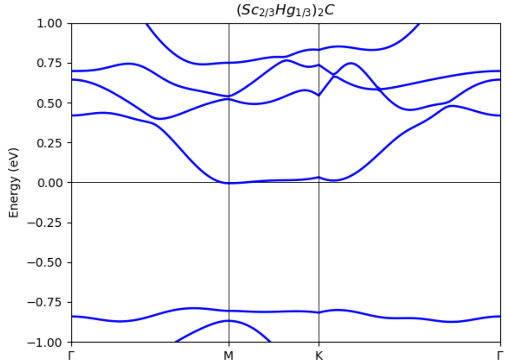
$(Sc_{2/3}Co_{1/3})_2C$



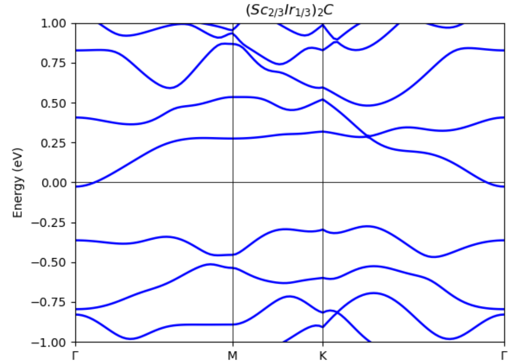
$(Sc_{2/3}Cu_{1/3})_2C$



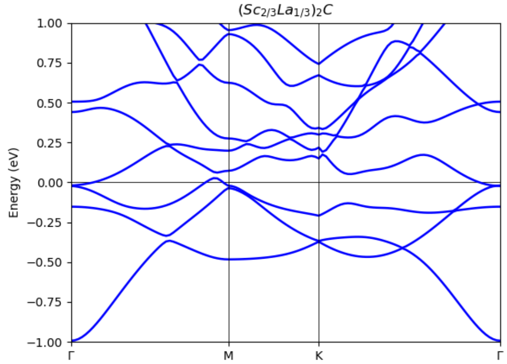
$(Sc_{2/3}Hg_{1/3})_2C$



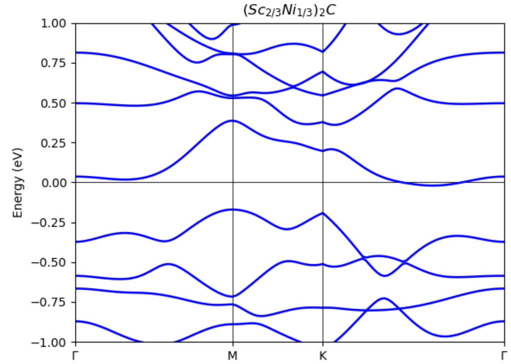
$(Sc_{2/3}Ir_{1/3})_2C$

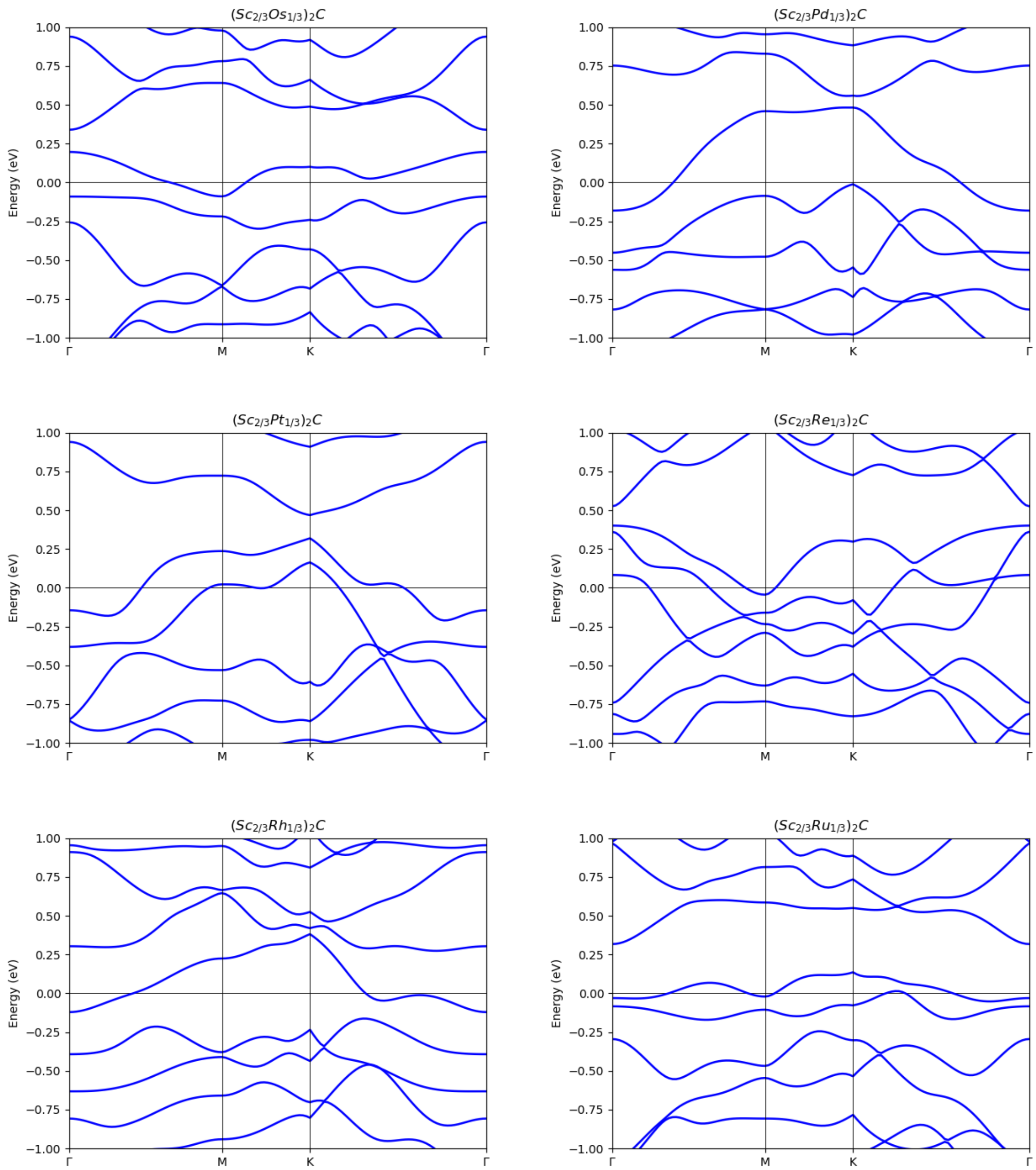


$(Sc_{2/3}La_{1/3})_2C$

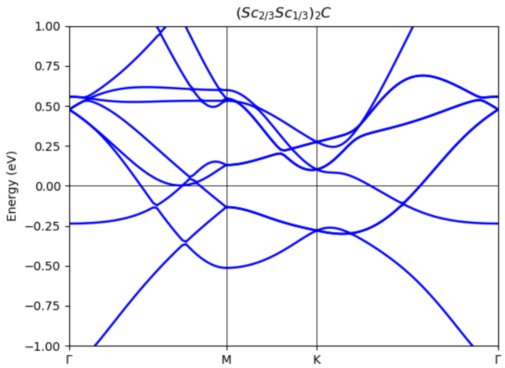


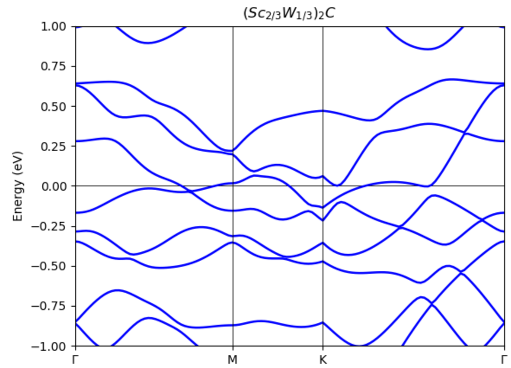
$(Sc_{2/3}Ni_{1/3})_2C$

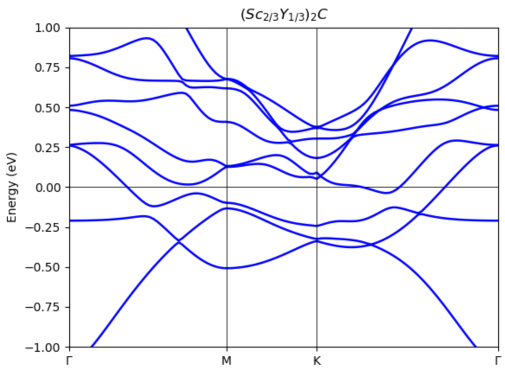


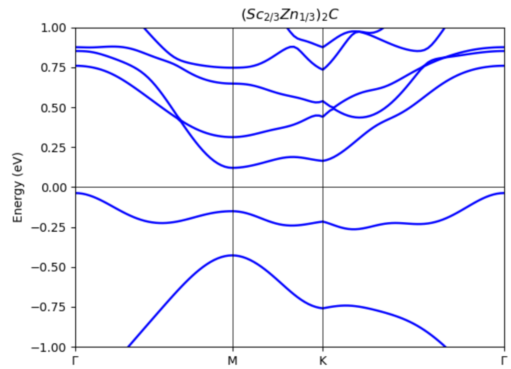


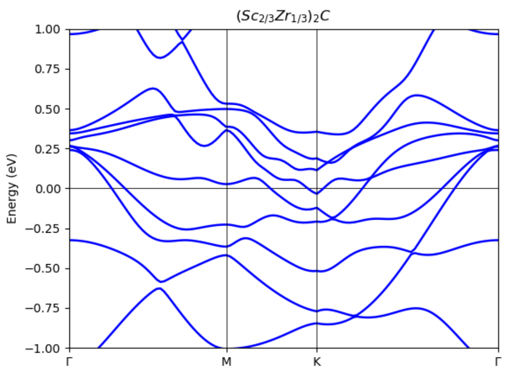
$(Sc_{2/3}Os_{1/3})_2C$
$(Sc_{2/3}Pd_{1/3})_2C$
$(Sc_{2/3}Pt_{1/3})_2C$
$(Sc_{2/3}Re_{1/3})_2C$
$(Sc_{2/3}Rh_{1/3})_2C$
$(Sc_{2/3}Ru_{1/3})_2C$
Energy (eV)
Γ M K Γ

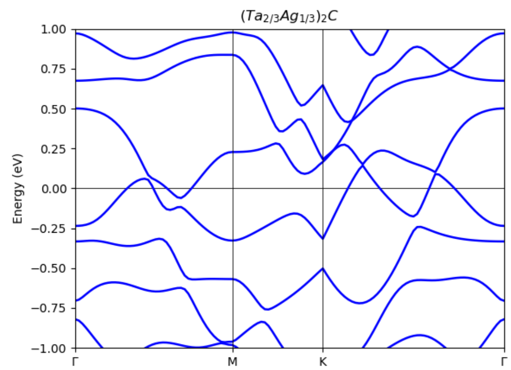

$(Sc_{2/3}Sc_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

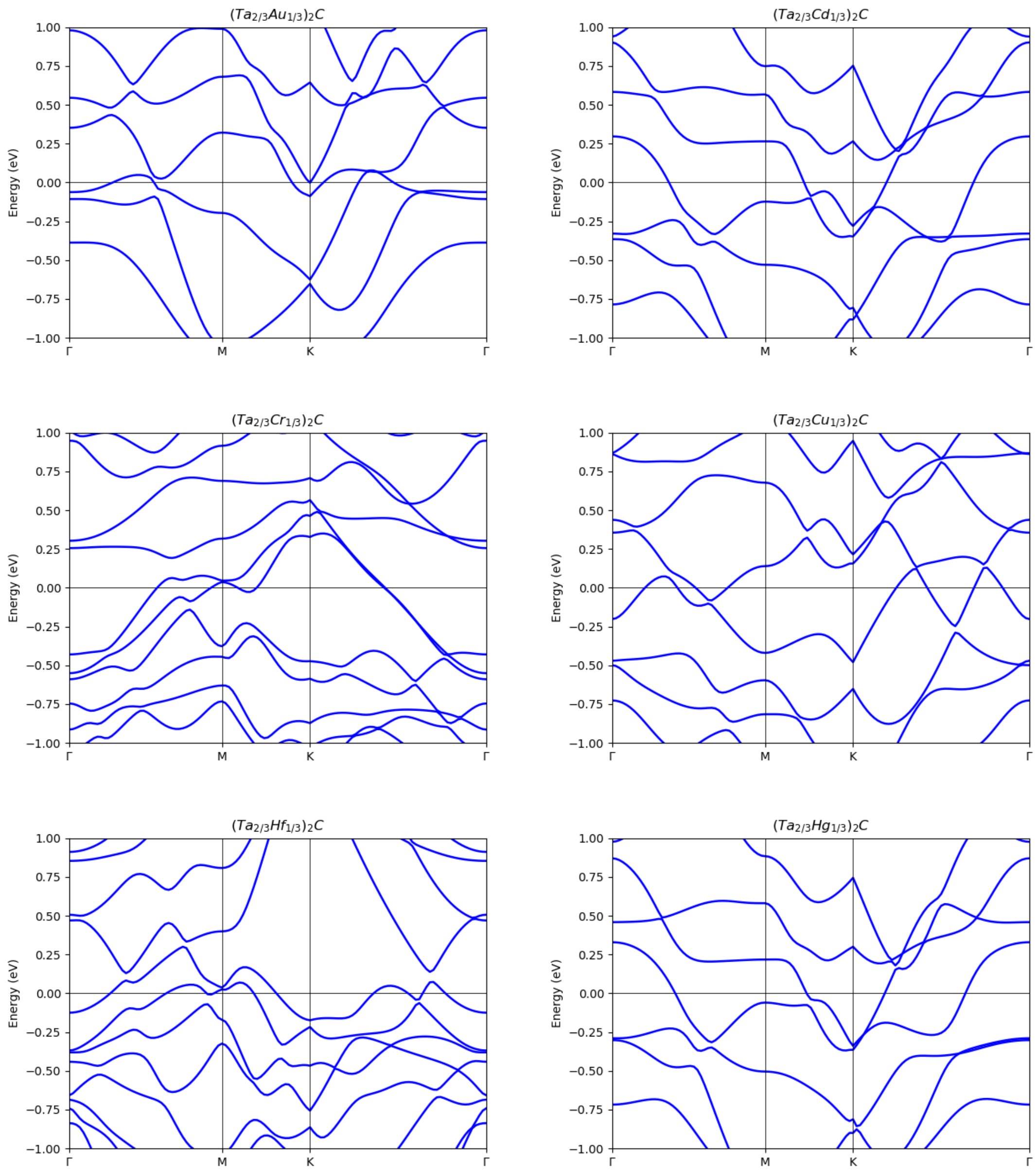

$(Sc_{2/3}W_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

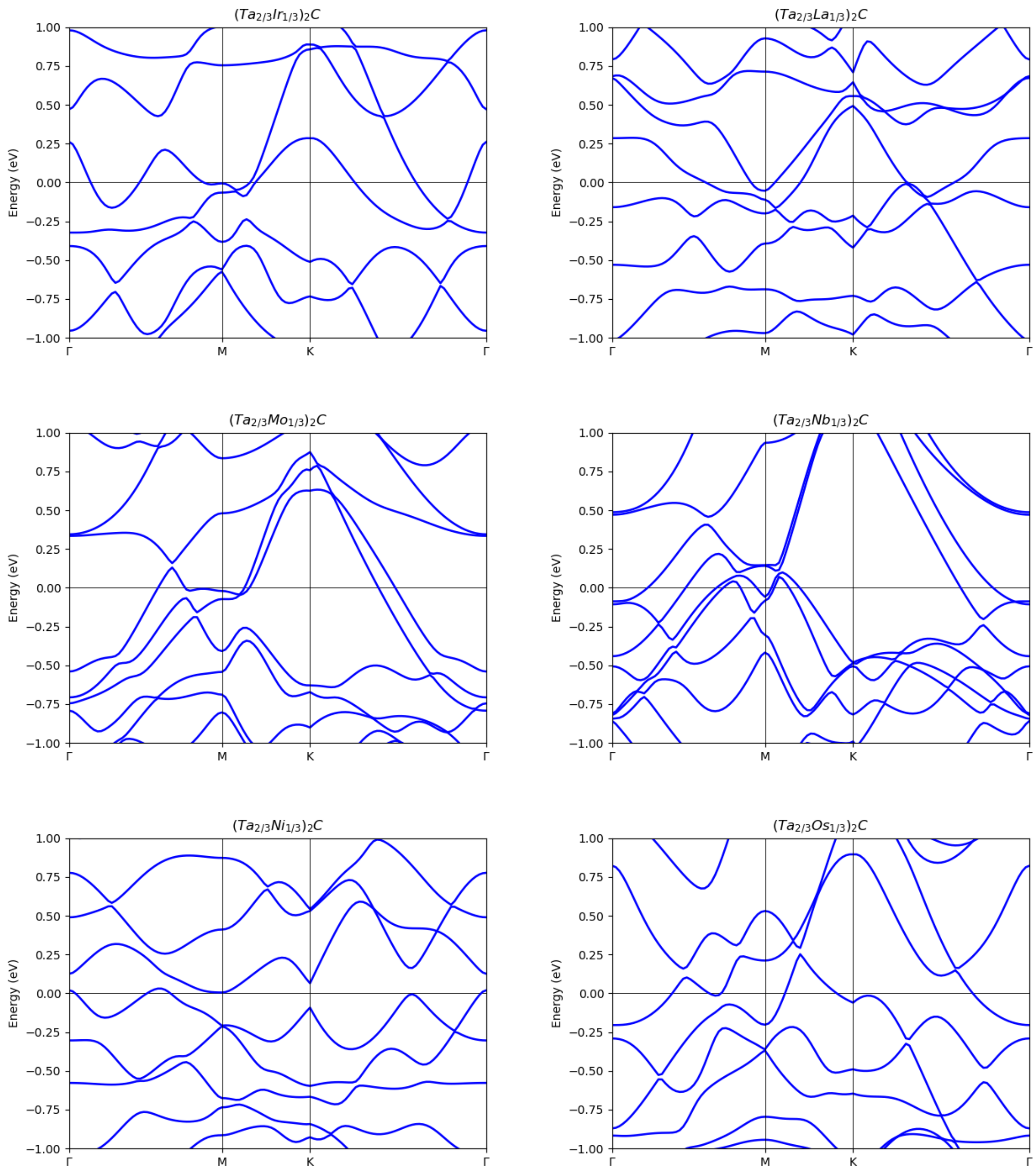

$(Sc_{2/3}Y_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

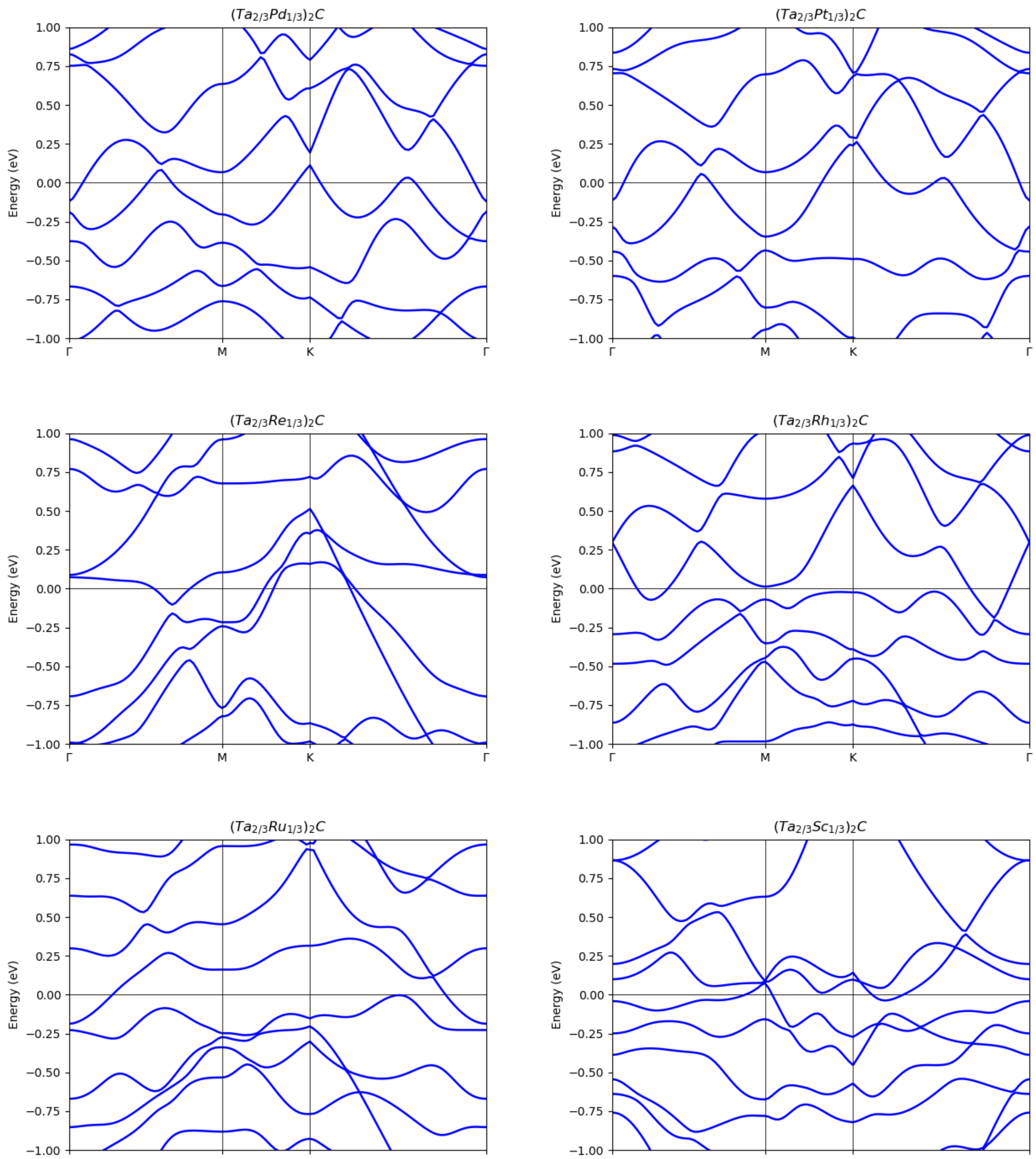

$(Sc_{2/3}Zn_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ


$(Sc_{2/3}Zr_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

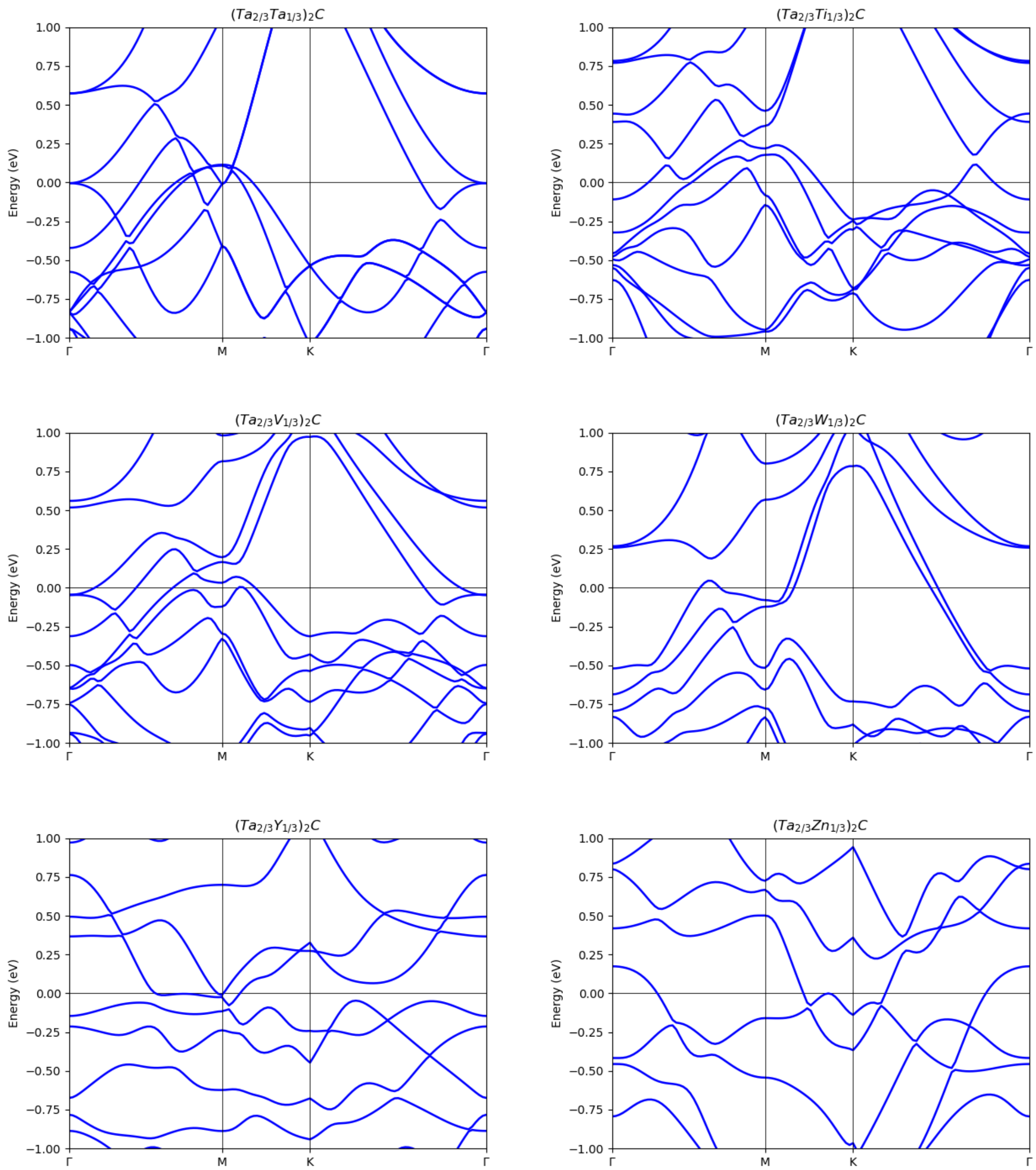

$(Ta_{2/3}Ag_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ


$(Ta_{2/3}Au_{1/3})_2C$
$(Ta_{2/3}Cd_{1/3})_2C$
$(Ta_{2/3}Cr_{1/3})_2C$
$(Ta_{2/3}Cu_{1/3})_2C$
$(Ta_{2/3}Hf_{1/3})_2C$
$(Ta_{2/3}Hg_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

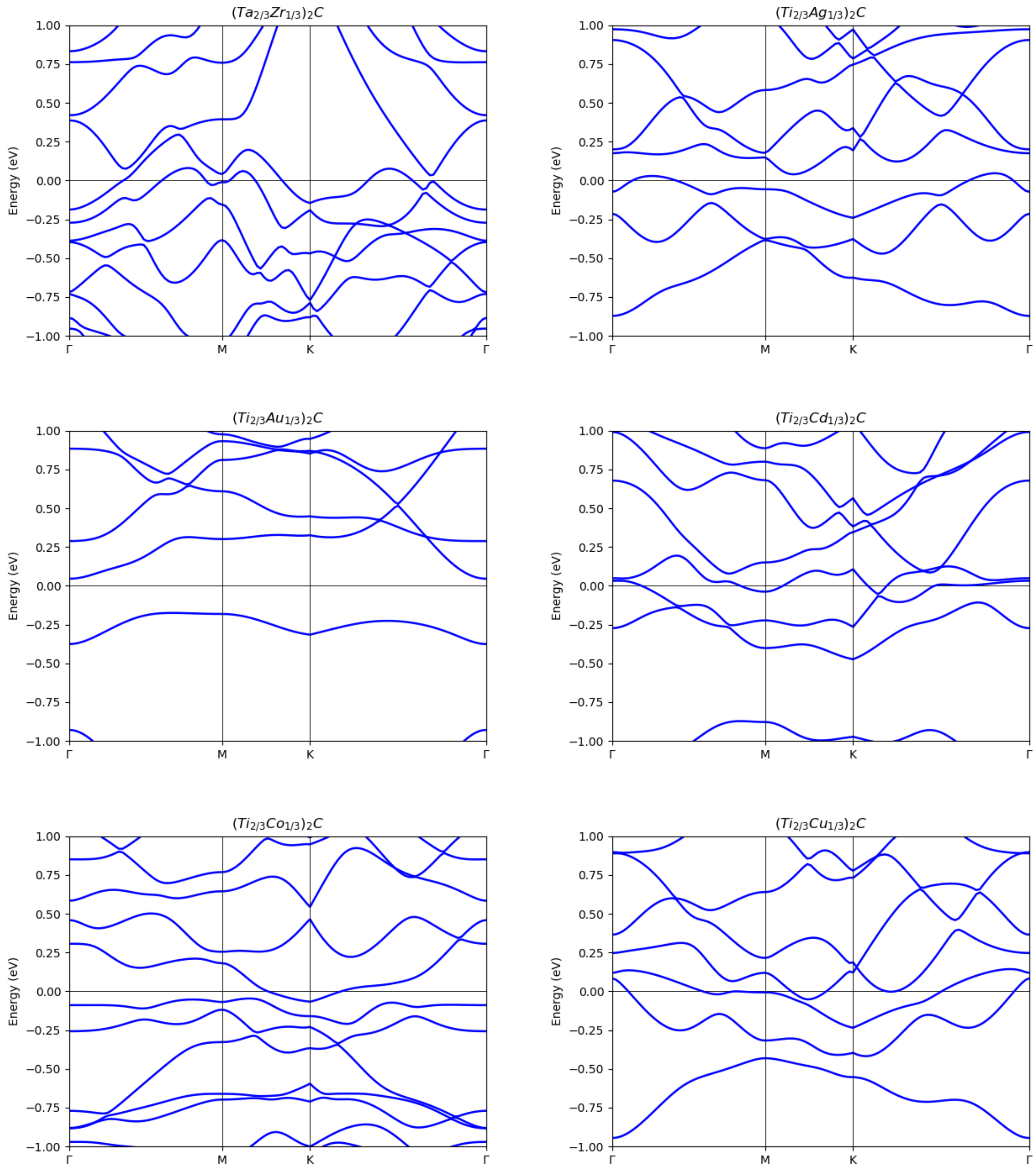

$(Ta_{2/3}Ir_{1/3})_2C$
$(Ta_{2/3}La_{1/3})_2C$
$(Ta_{2/3}Mo_{1/3})_2C$
$(Ta_{2/3}Nb_{1/3})_2C$
$(Ta_{2/3}Ni_{1/3})_2C$
$(Ta_{2/3}Os_{1/3})_2C$
Energy (eV)
Γ M K Γ

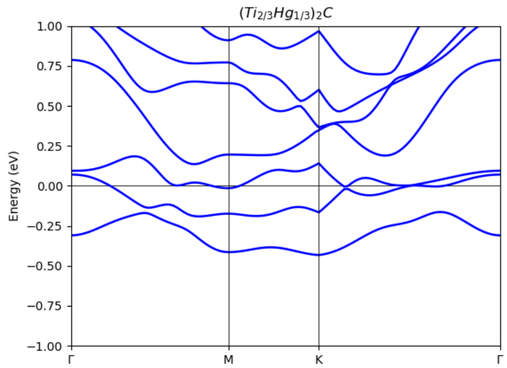


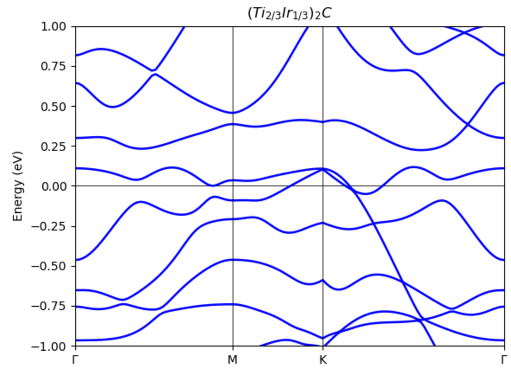
$(Ta_{2/3}Pd_{1/3})_2C$
$(Ta_{2/3}Pt_{1/3})_2C$
$(Ta_{2/3}Re_{1/3})_2C$
$(Ta_{2/3}Rh_{1/3})_2C$
$(Ta_{2/3}Ru_{1/3})_2C$
$(Ta_{2/3}Sc_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

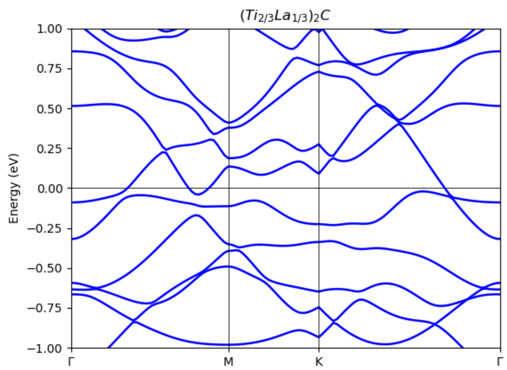


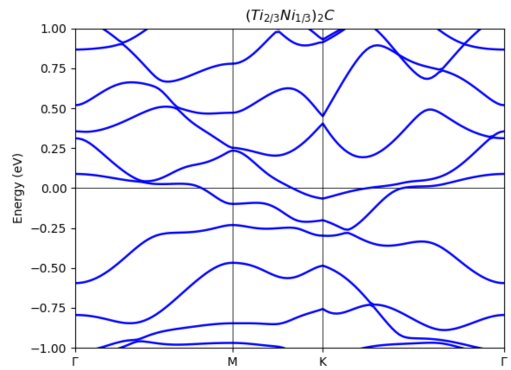
$(Ta_{2/3}Ta_{1/3})_2C$
$(Ta_{2/3}Ti_{1/3})_2C$
$(Ta_{2/3}V_{1/3})_2C$
$(Ta_{2/3}W_{1/3})_2C$
$(Ta_{2/3}Y_{1/3})_2C$
$(Ta_{2/3}Zn_{1/3})_2C$
Energy (eV)
Γ M K Γ

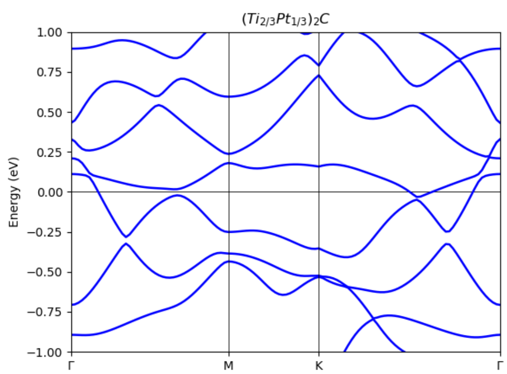

$(Ta_{2/3}Zr_{1/3})_2C$
$(Ti_{2/3}Ag_{1/3})_2C$
$(Ti_{2/3}Au_{1/3})_2C$
$(Ti_{2/3}Cd_{1/3})_2C$
$(Ti_{2/3}Co_{1/3})_2C$
$(Ti_{2/3}Cu_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

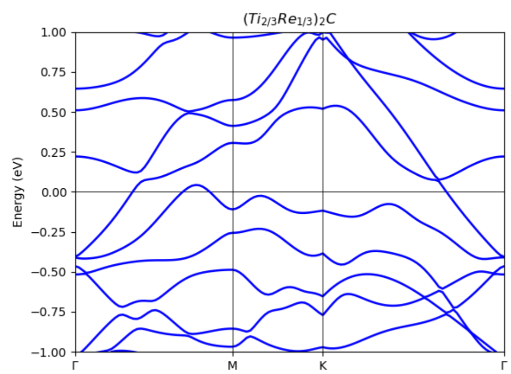

$(Ti_{2/3}Hg_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

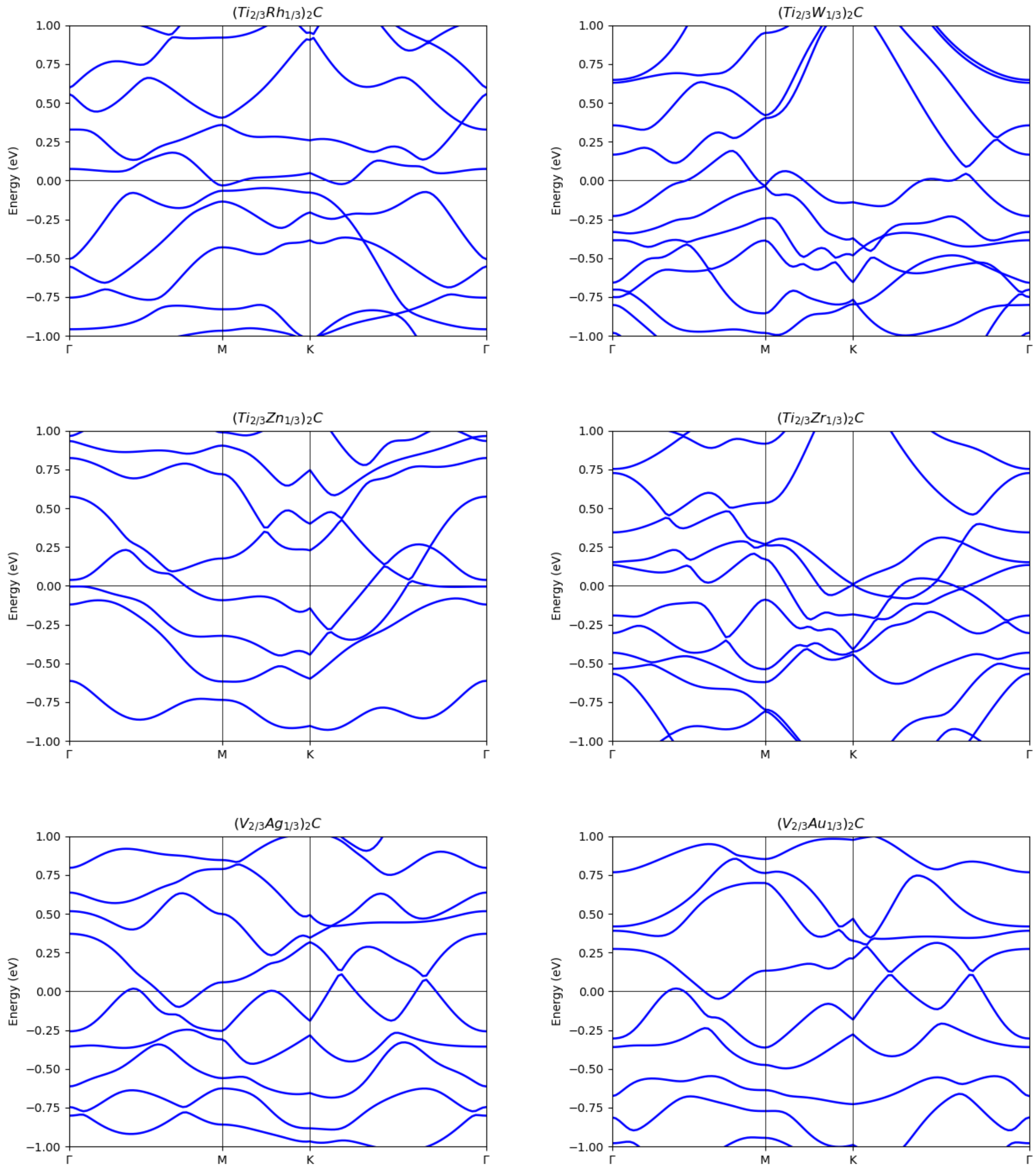

$(Ti_{2/3}Ir_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ


$(Ti_{2/3}La_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

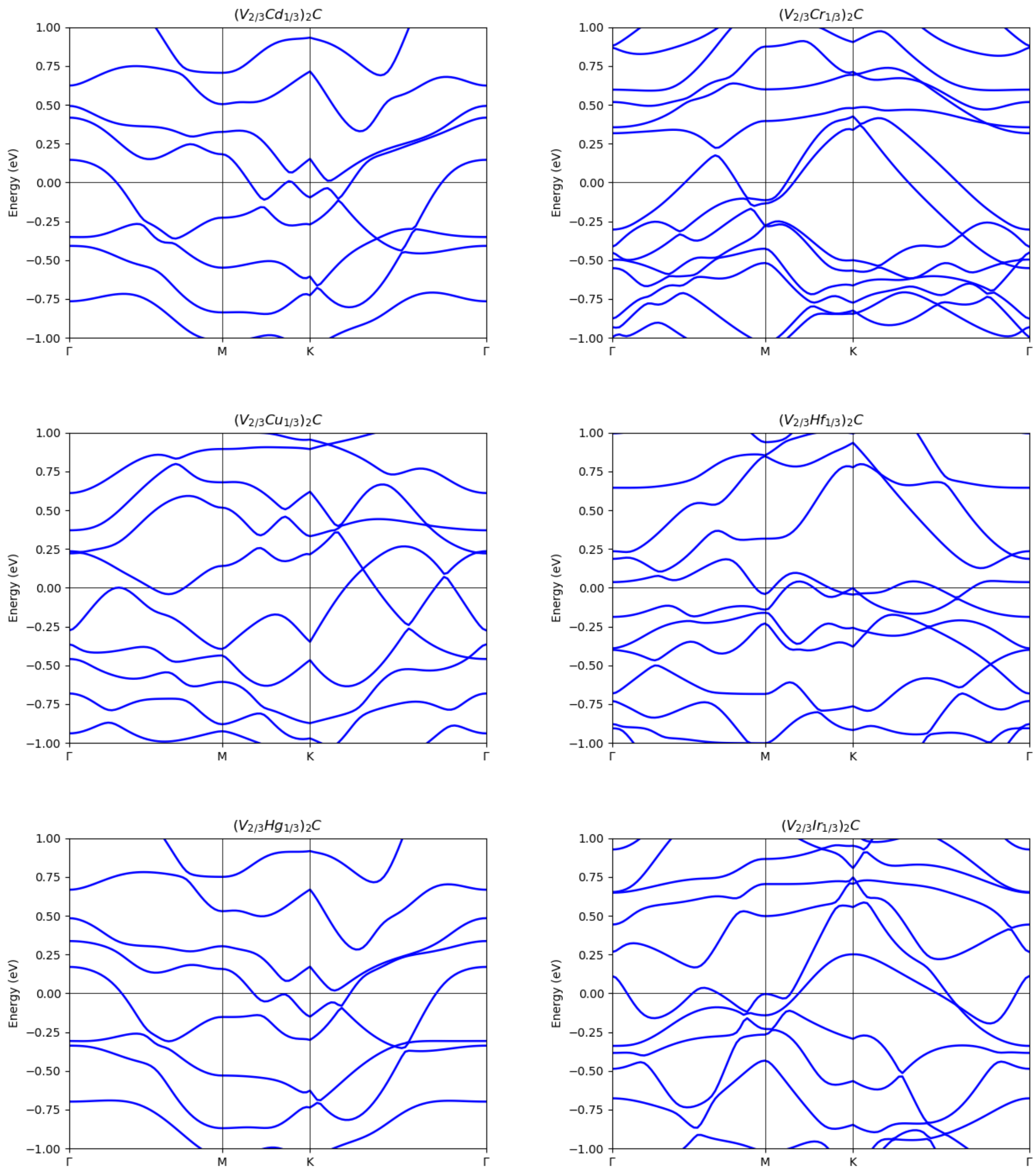

$(Ti_{2/3}Ni_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

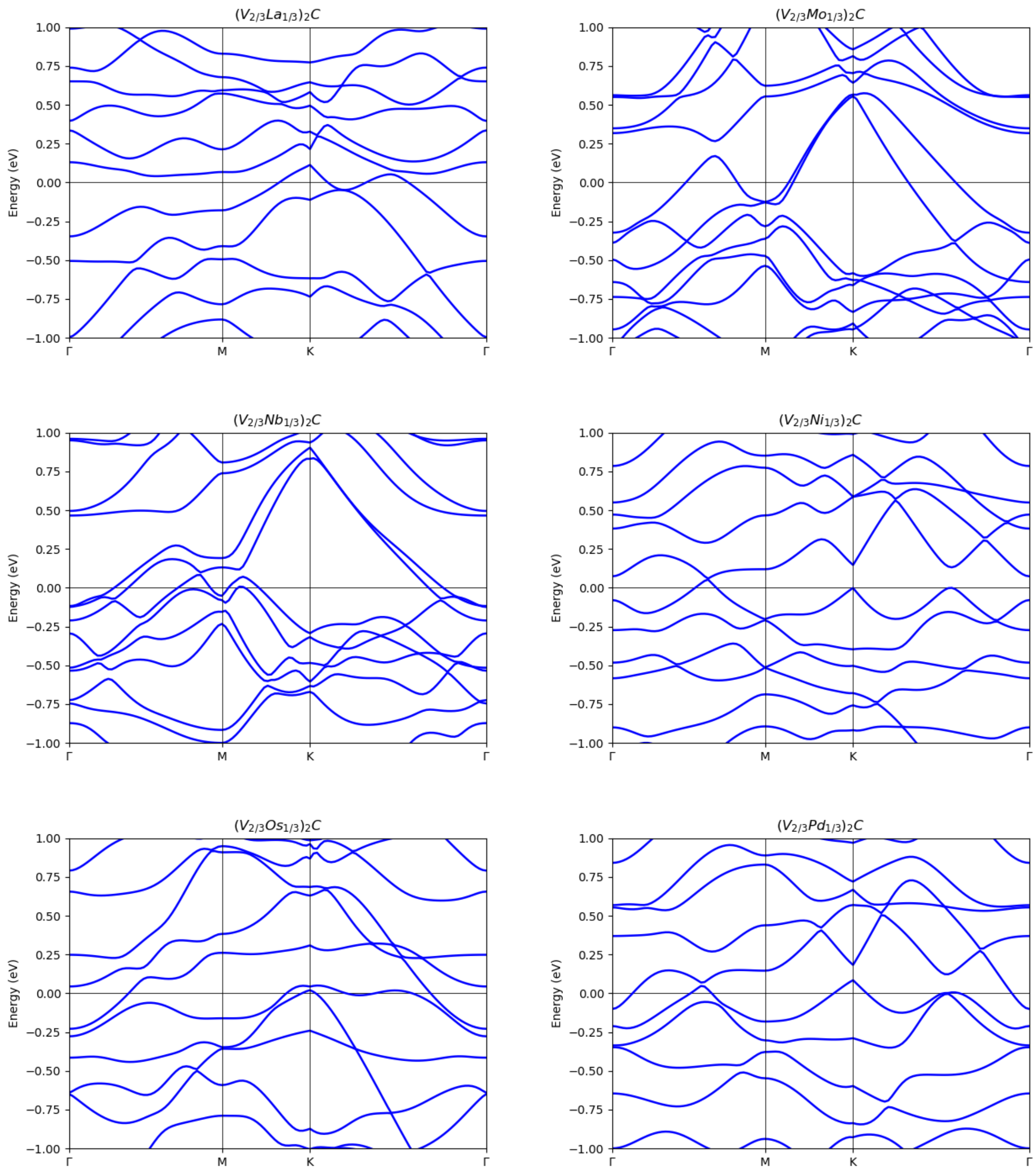

$(Ti_{2/3}Pt_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

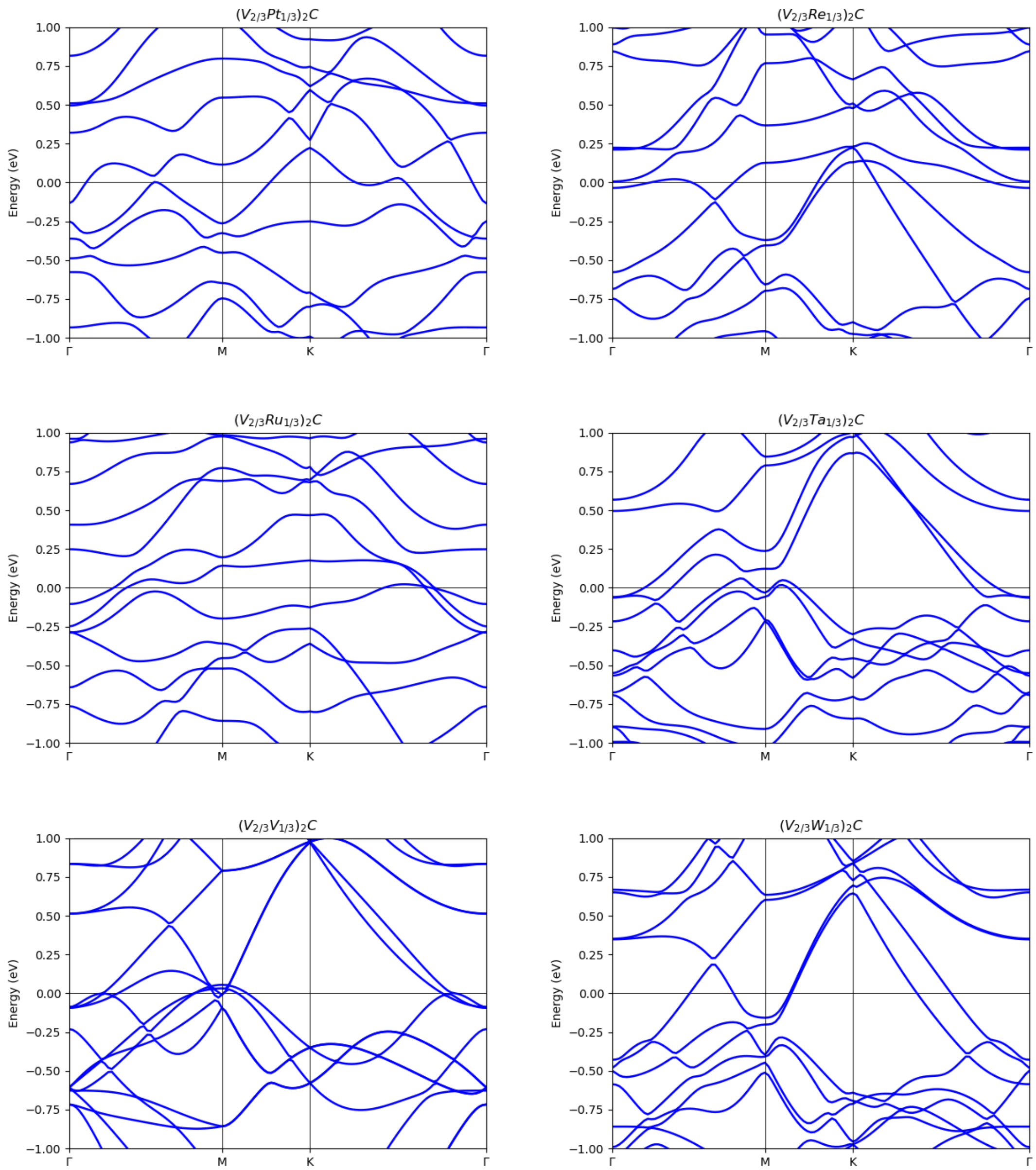

$(Ti_{2/3}Re_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

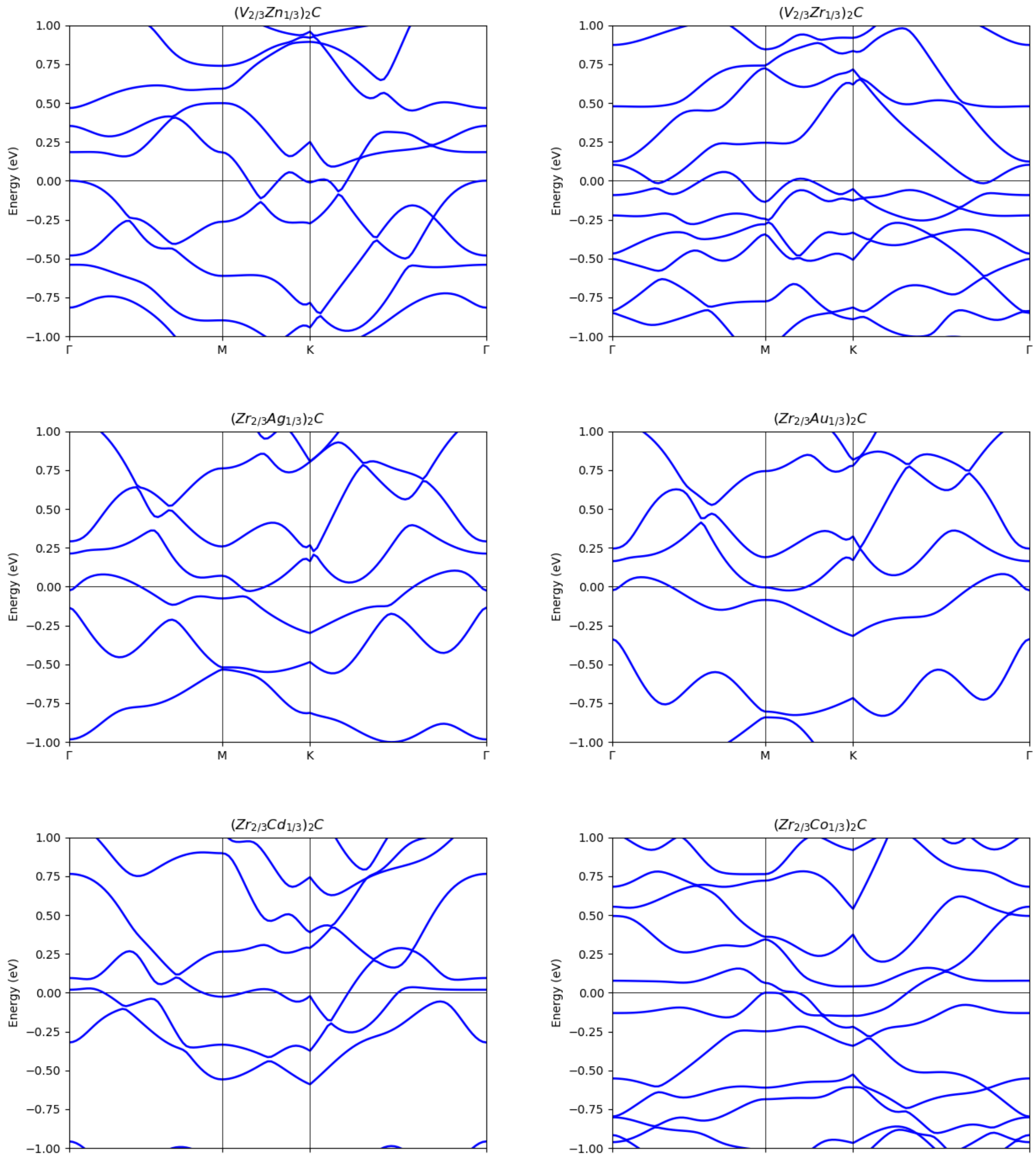


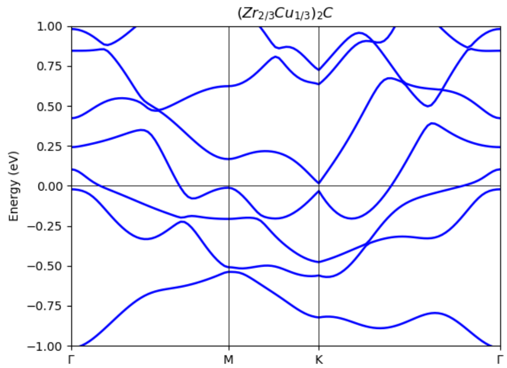
$(Ti_{2/3}Rh_{1/3})_2C$
$(Ti_{2/3}W_{1/3})_2C$
$(Ti_{2/3}Zn_{1/3})_2C$
$(Ti_{2/3}Zr_{1/3})_2C$
$(V_{2/3}Ag_{1/3})_2C$
$(V_{2/3}Au_{1/3})_2C$
Energy (eV)
Γ M K Γ

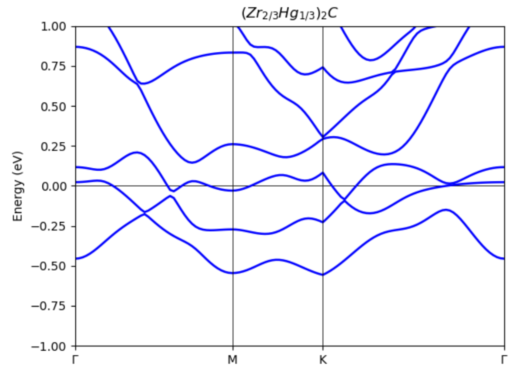

$(V_{2/3}Cd_{1/3})_2C$
$(V_{2/3}Cr_{1/3})_2C$
$(V_{2/3}Cu_{1/3})_2C$
$(V_{2/3}Hf_{1/3})_2C$
$(V_{2/3}Hg_{1/3})_2C$
$(V_{2/3}Ir_{1/3})_2C$
Energy (eV)
Γ M K Γ

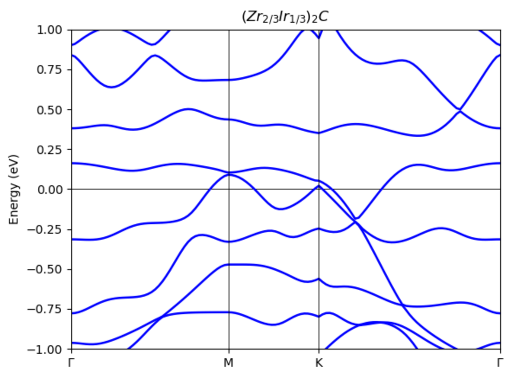

$(V_{2/3}La_{1/3})_2C$
$(V_{2/3}Mo_{1/3})_2C$
$(V_{2/3}Nb_{1/3})_2C$
$(V_{2/3}Ni_{1/3})_2C$
$(V_{2/3}Os_{1/3})_2C$
$(V_{2/3}Pd_{1/3})_2C$
Energy (eV)
Γ
M
K

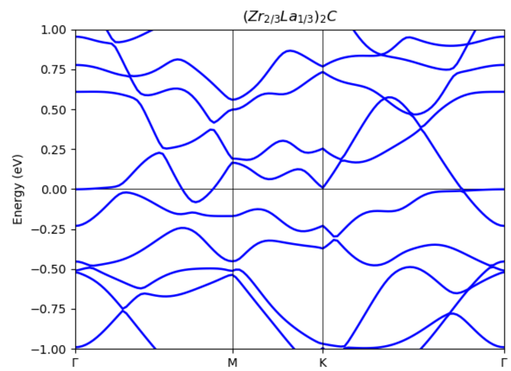

$(V_{2/3}Pt_{1/3})_2C$
$(V_{2/3}Re_{1/3})_2C$
$(V_{2/3}Ru_{1/3})_2C$
$(V_{2/3}Ta_{1/3})_2C$
$(V_{2/3}V_{1/3})_2C$
$(V_{2/3}W_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

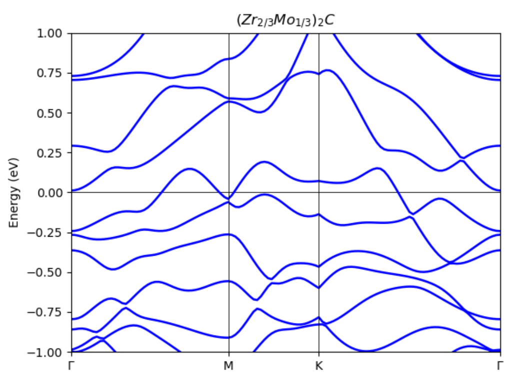

$(V_{2/3}Zn_{1/3})_2C$
$(V_{2/3}Zr_{1/3})_2C$
$(Zr_{2/3}Ag_{1/3})_2C$
$(Zr_{2/3}Au_{1/3})_2C$
$(Zr_{2/3}Cd_{1/3})_2C$
$(Zr_{2/3}Co_{1/3})_2C$
Energy (eV)
Γ
M
K
Γ

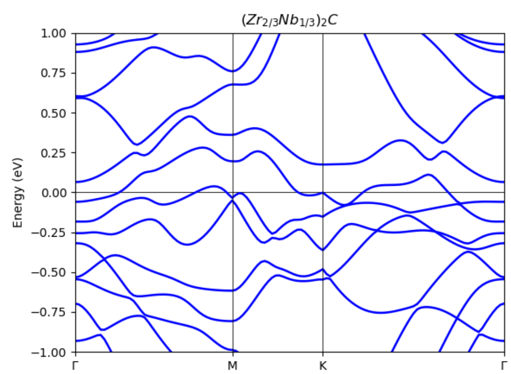

$(Zr_{2/3}Cu_{1/3})_2C$
Energy (eV)
Γ M K Γ

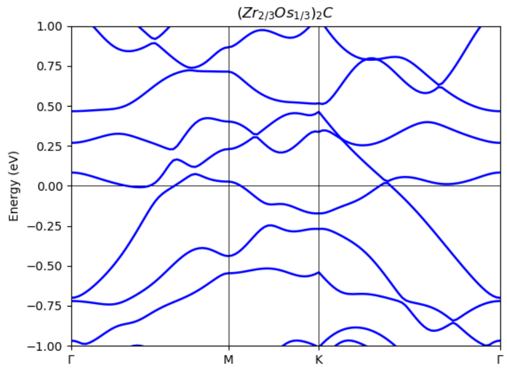

$(Zr_{2/3}Hg_{1/3})_2C$
Energy (eV)
Γ M K Γ

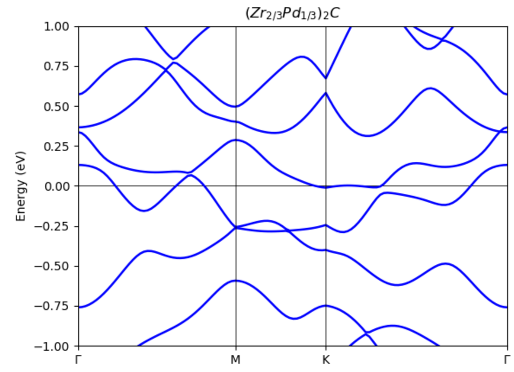

$(Zr_{2/3}Ir_{1/3})_2C$
Energy (eV)
Γ M K Γ

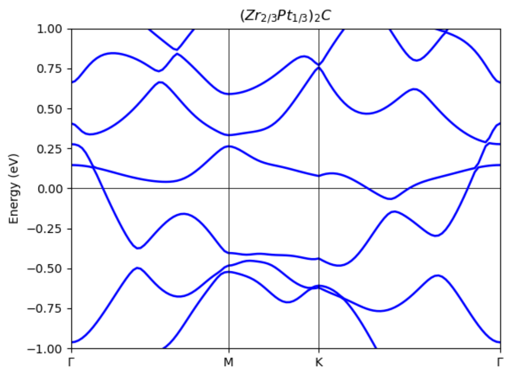

$(Zr_{2/3}La_{1/3})_2C$
Energy (eV)
Γ M K Γ

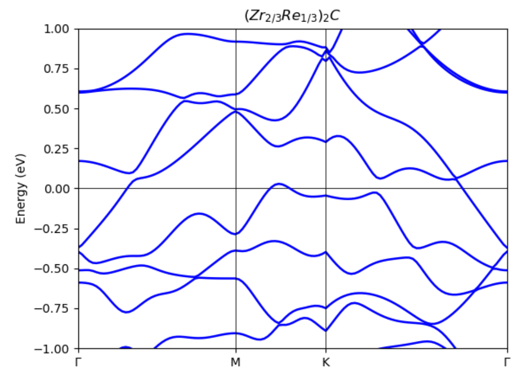

$(Zr_{2/3}Mo_{1/3})_2C$
Energy (eV)
Γ M K Γ

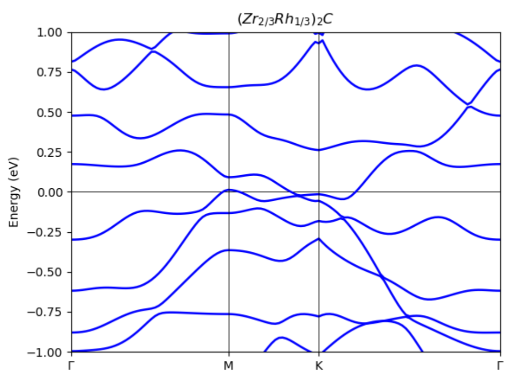

$(Zr_{2/3}Nb_{1/3})_2C$
Energy (eV)
Γ M K Γ

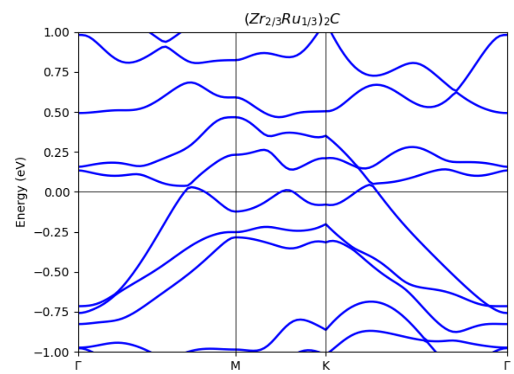

$(Zr_{2/3}Os_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

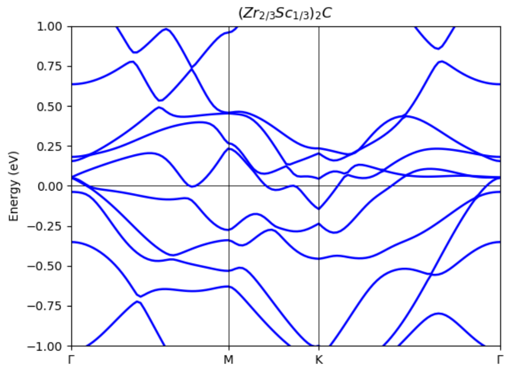

$(Zr_{2/3}Pd_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

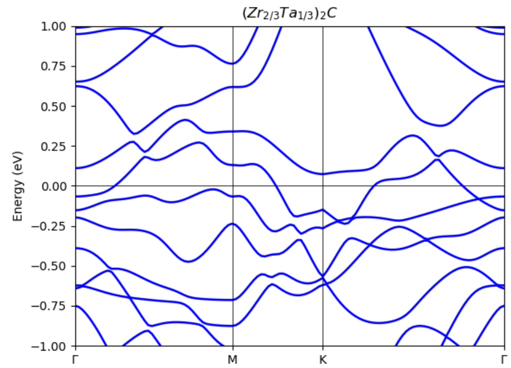

$(Zr_{2/3}Pt_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

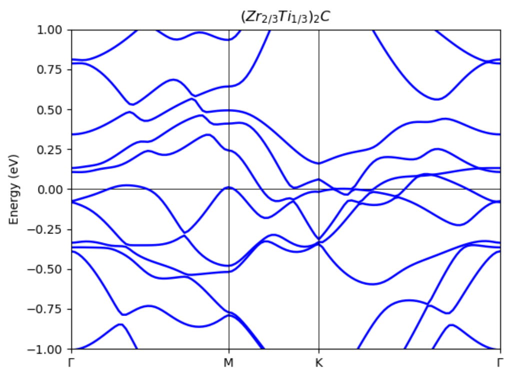

$(Zr_{2/3}Re_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

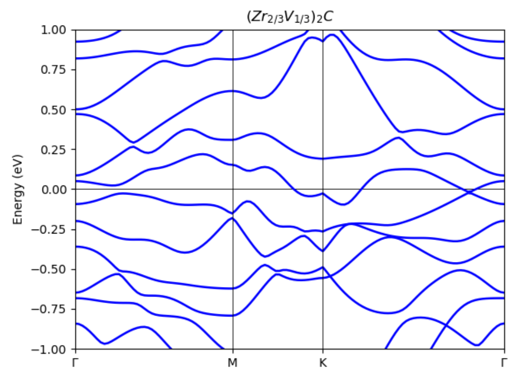

$(Zr_{2/3}Rh_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

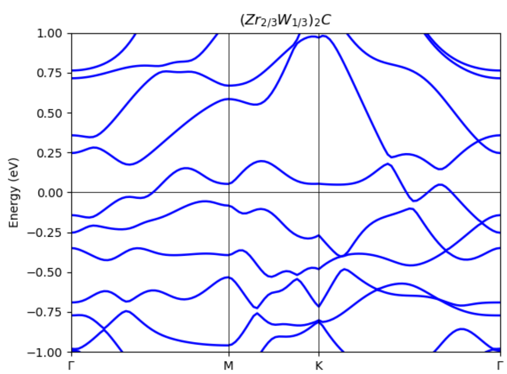

$(Zr_{2/3}Ru_{1/3})_2C$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

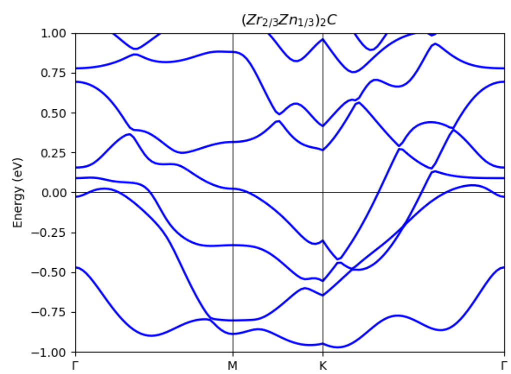

$(Zr_{2/3}Sc_{1/3})_2C$
Energy (eV)
Γ M K Γ

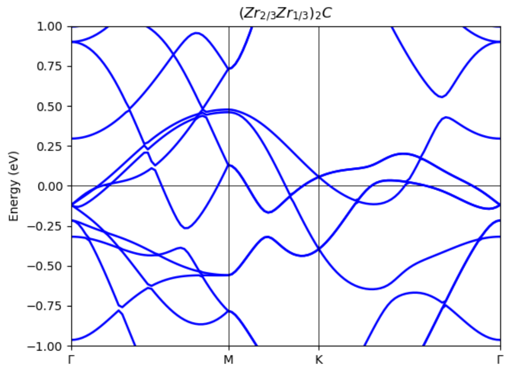

$(Zr_{2/3}Ta_{1/3})_2C$
Energy (eV)
Γ M K Γ

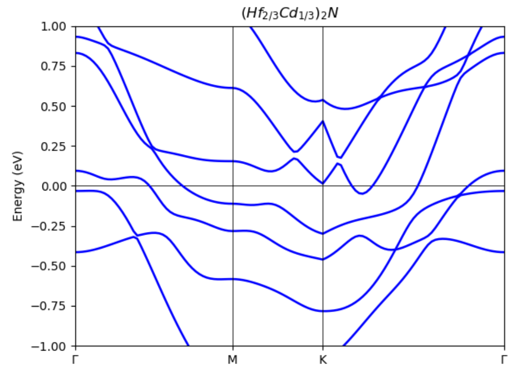

$(Zr_{2/3}Ti_{1/3})_2C$
Energy (eV)
Γ M K Γ

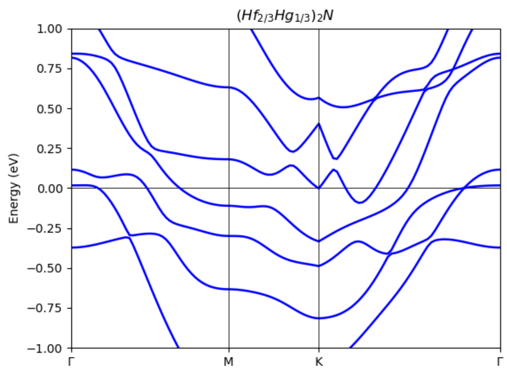

$(Zr_{2/3}V_{1/3})_2C$
Energy (eV)
Γ M K Γ

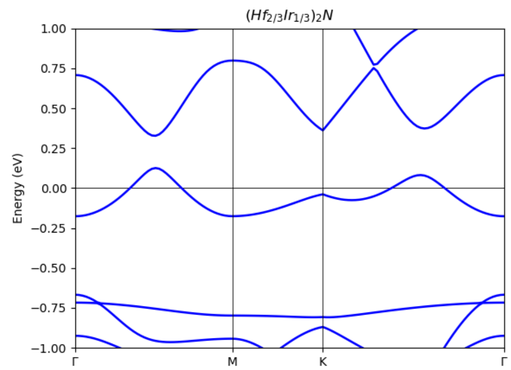

$(Zr_{2/3}W_{1/3})_2C$
Energy (eV)
Γ M K Γ

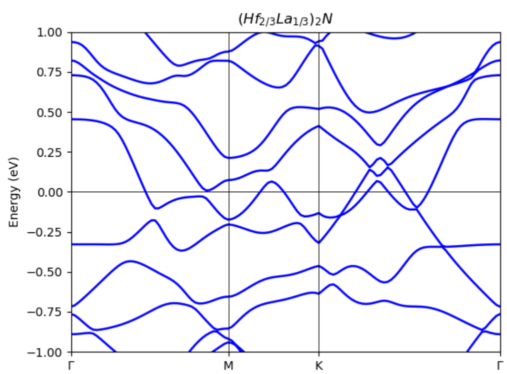

$(Zr_{2/3}Zn_{1/3})_2C$
Energy (eV)
Γ M K Γ

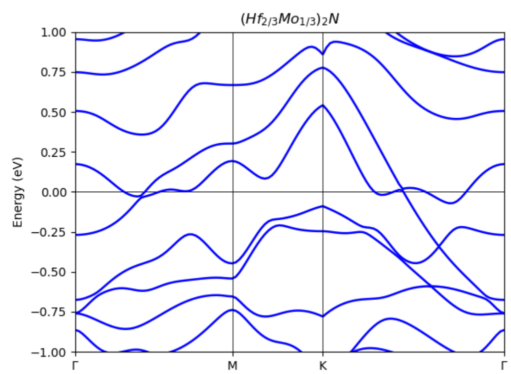

$(Zr_{2/3}Zr_{1/3})_2C$
Energy (eV)
Γ M K Γ

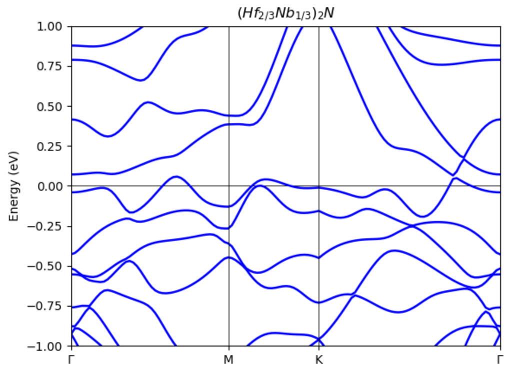

$(Hf_{2/3}Cd_{1/3})_2N$
Energy (eV)
Γ M K Γ

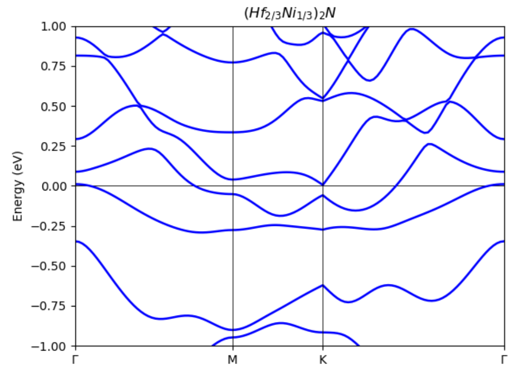

$(Hf_{2/3}Hg_{1/3})_2N$
Energy (eV)
Γ M K Γ

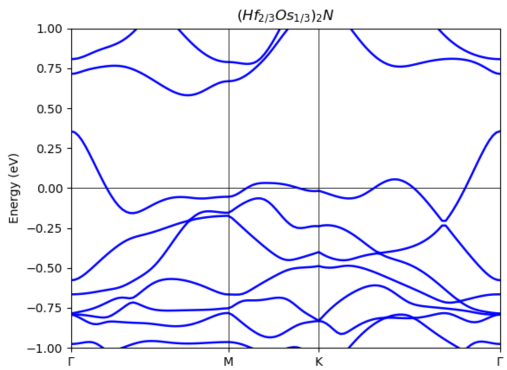

$(Hf_{2/3}Ir_{1/3})_2N$
Energy (eV)
Γ M K Γ

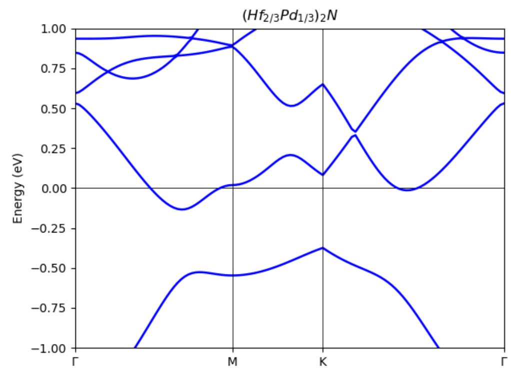

$(Hf_{2/3}La_{1/3})_2N$
Energy (eV)
Γ M K Γ

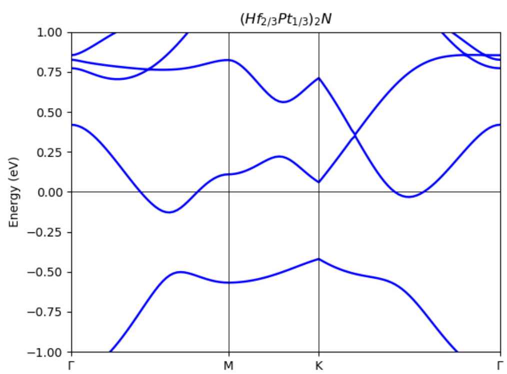

$(Hf_{2/3}Mo_{1/3})_2N$
Energy (eV)
Γ M K Γ

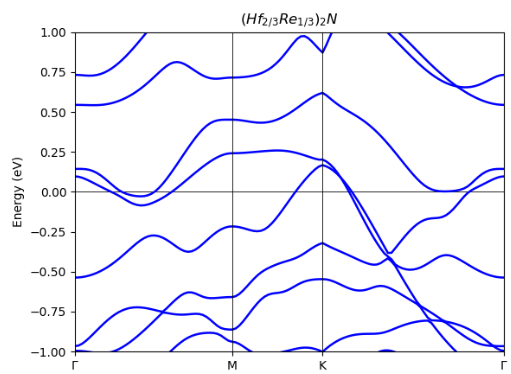

$(Hf_{2/3}Nb_{1/3})_2N$
Energy (eV)
Γ M K Γ

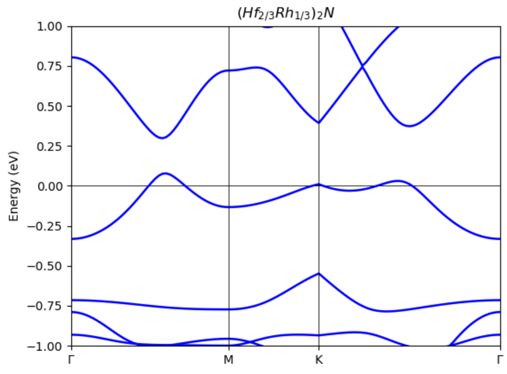

$(Hf_{2/3}Ni_{1/3})_2N$
Energy (eV)
Γ M K Γ

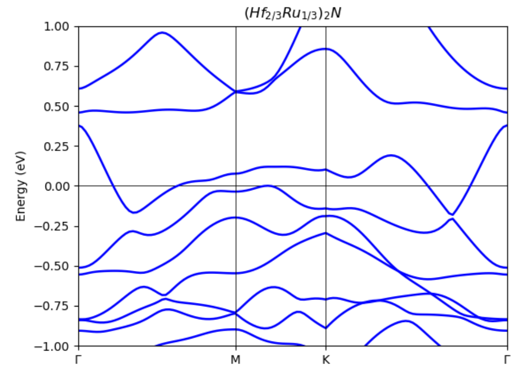

$(Hf_{2/3}Os_{1/3})_2N$
Energy (eV)
Γ M K Γ

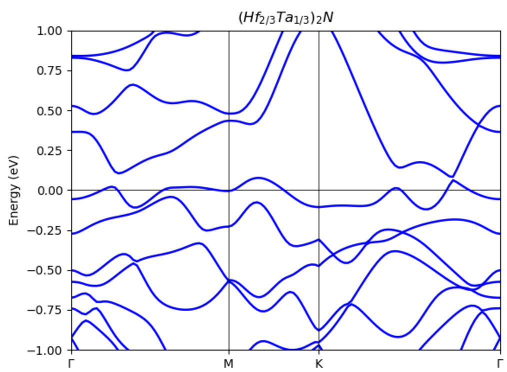

$(Hf_{2/3}Pd_{1/3})_2N$
Energy (eV)
Γ M K Γ

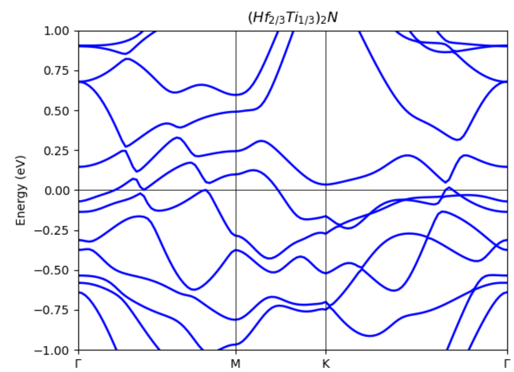

$(Hf_{2/3}Pt_{1/3})_2N$
Energy (eV)
Γ M K Γ

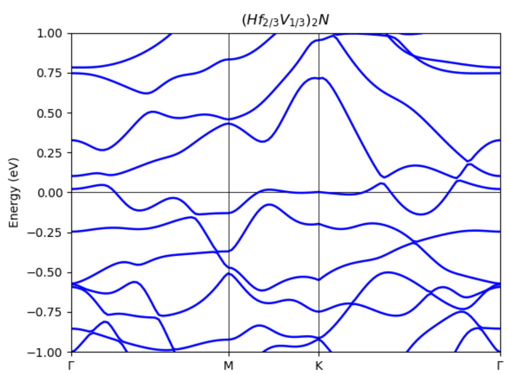

$(Hf_{2/3}Re_{1/3})_2N$
Energy (eV)
Γ M K Γ

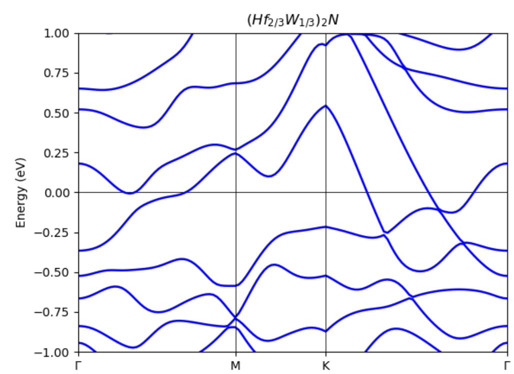

$(Hf_{2/3}Rh_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

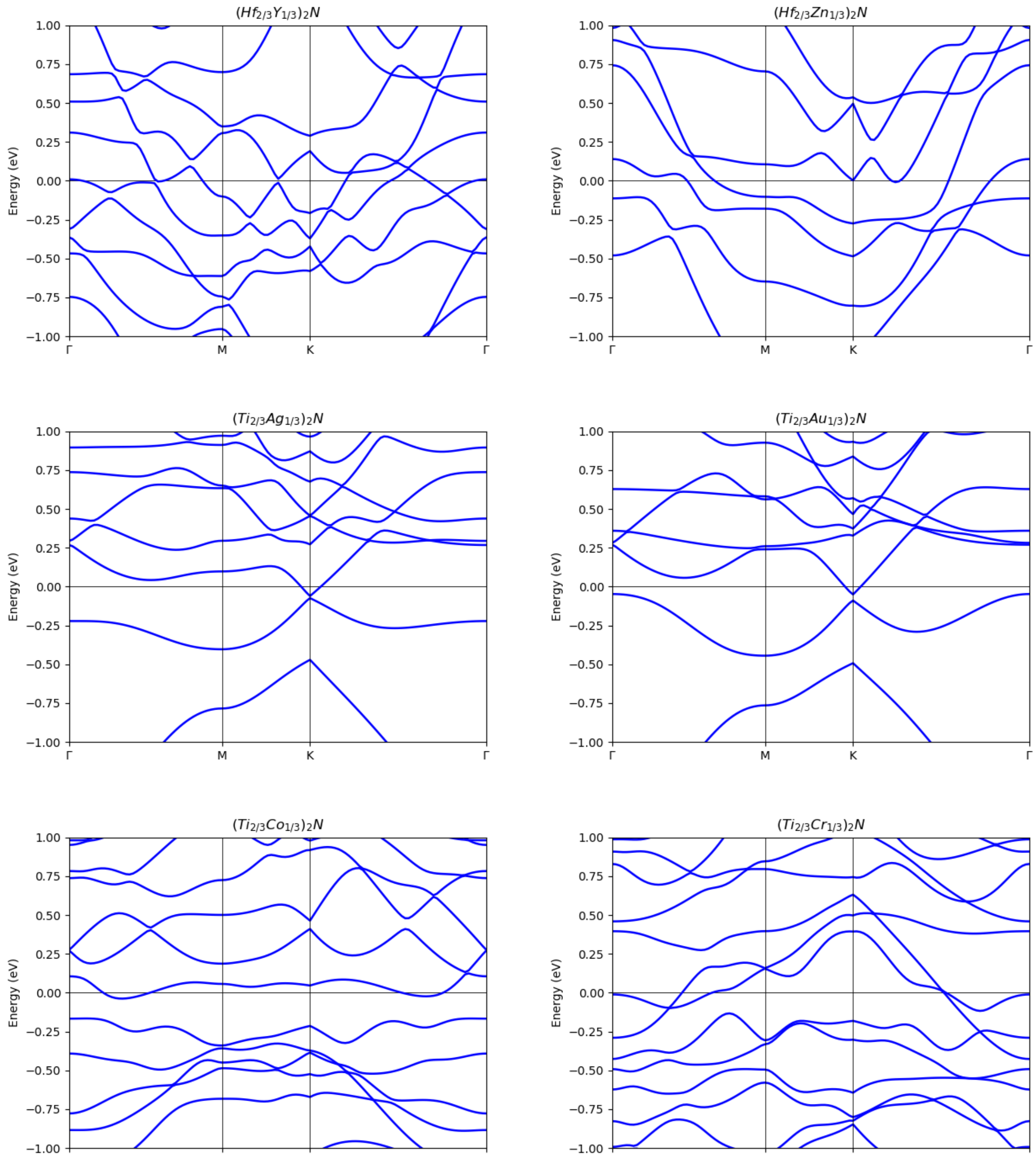

$(Hf_{2/3}Ru_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

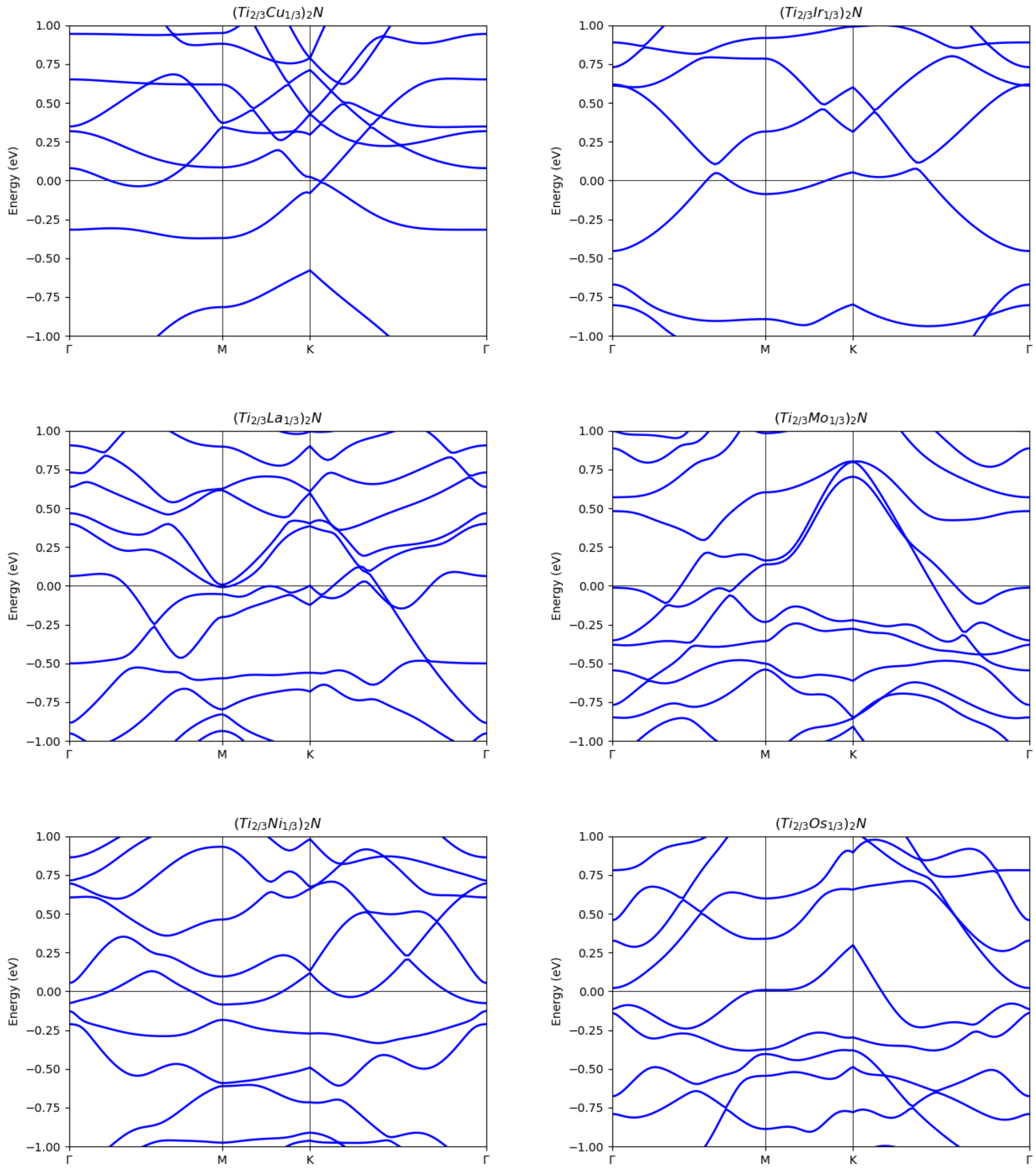

$(Hf_{2/3}Ta_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

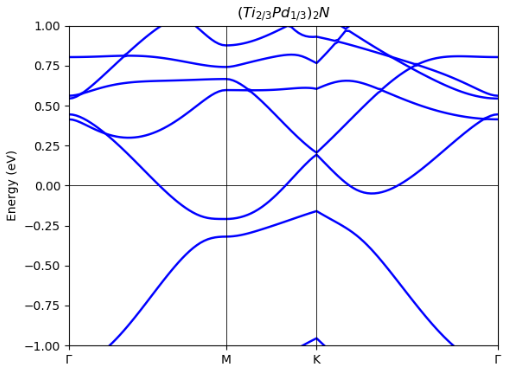

$(Hf_{2/3}Ti_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

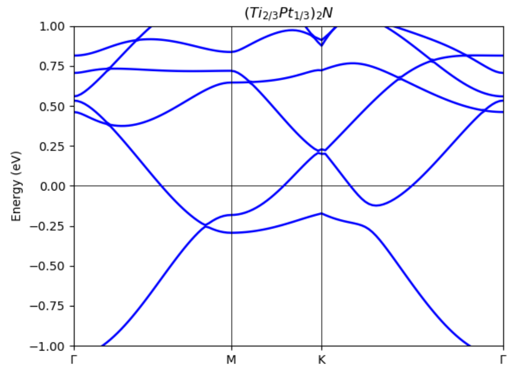

$(Hf_{2/3}V_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

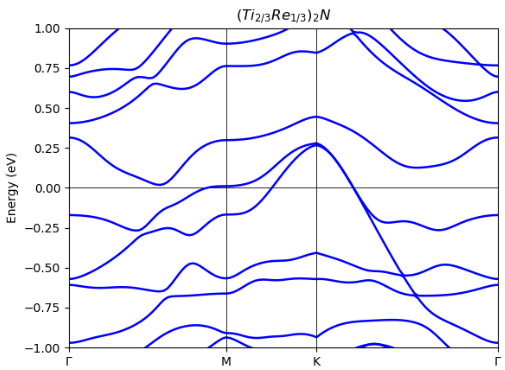

$(Hf_{2/3}W_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

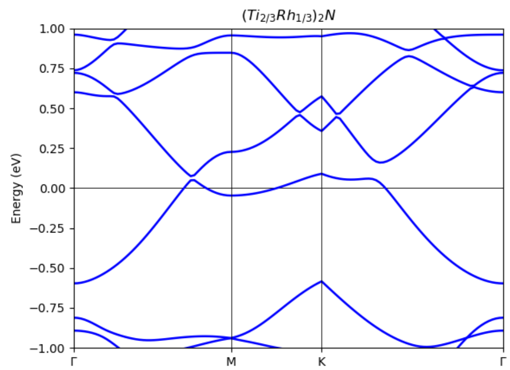

$(Hf_{2/3}Y_{1/3})_2N$
$(Hf_{2/3}Zn_{1/3})_2N$
$(Ti_{2/3}Ag_{1/3})_2N$
$(Ti_{2/3}Au_{1/3})_2N$
$(Ti_{2/3}Co_{1/3})_2N$
$(Ti_{2/3}Cr_{1/3})_2N$
Energy (eV)
Γ
M
K

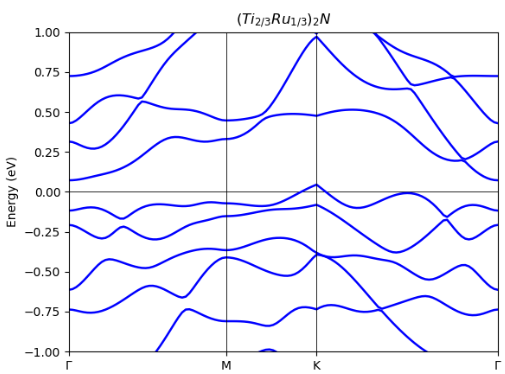

$(Ti_{2/3}Cu_{1/3})_2N$
$(Ti_{2/3}Ir_{1/3})_2N$
$(Ti_{2/3}La_{1/3})_2N$
$(Ti_{2/3}Mo_{1/3})_2N$
$(Ti_{2/3}Ni_{1/3})_2N$
$(Ti_{2/3}Os_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ

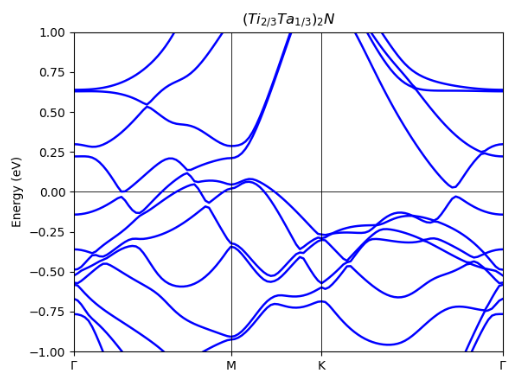

$(Ti_{2/3}Pd_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

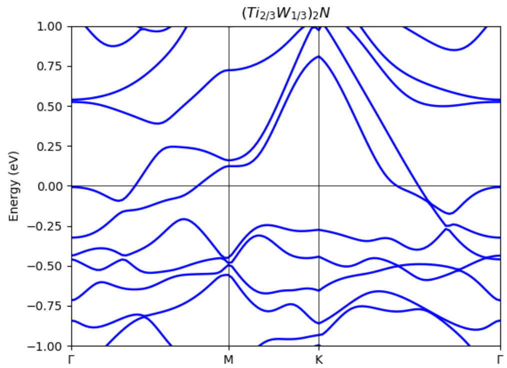

$(Ti_{2/3}Pt_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

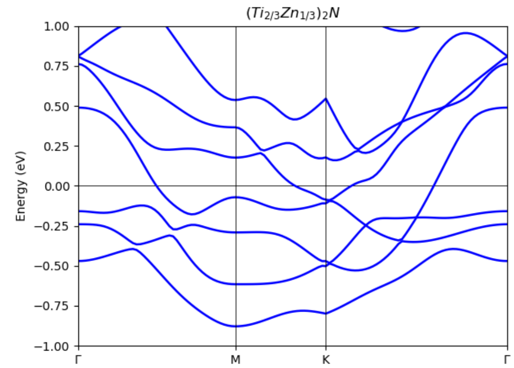

$(Ti_{2/3}Re_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

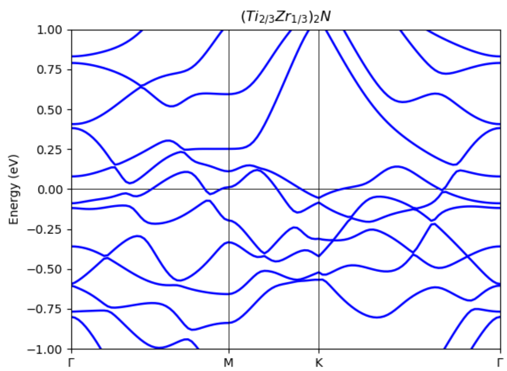

$(Ti_{2/3}Rh_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

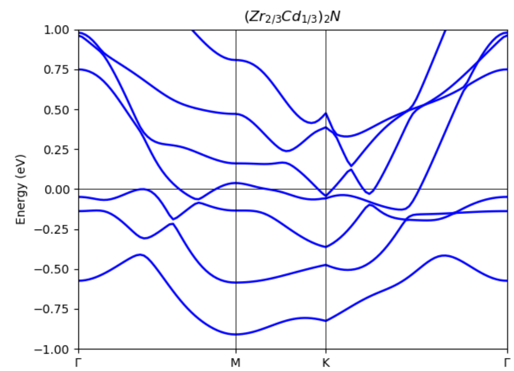

$(Ti_{2/3}Ru_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

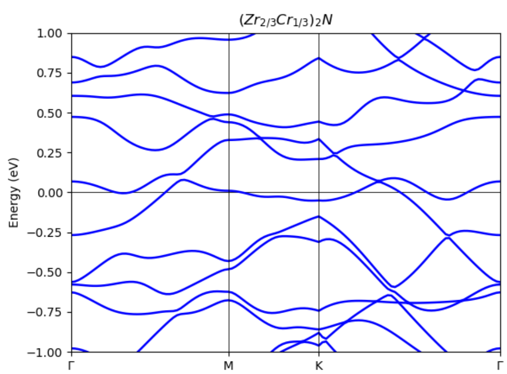

$(Ti_{2/3}Ta_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

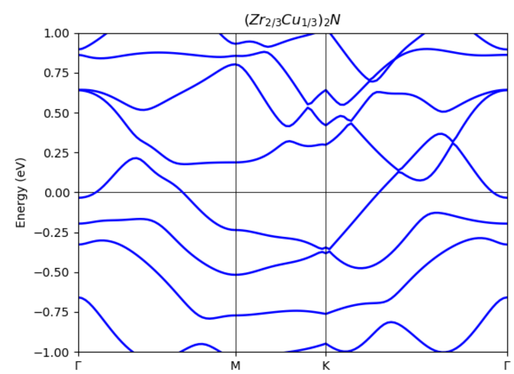

$(Ti_{2/3}W_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

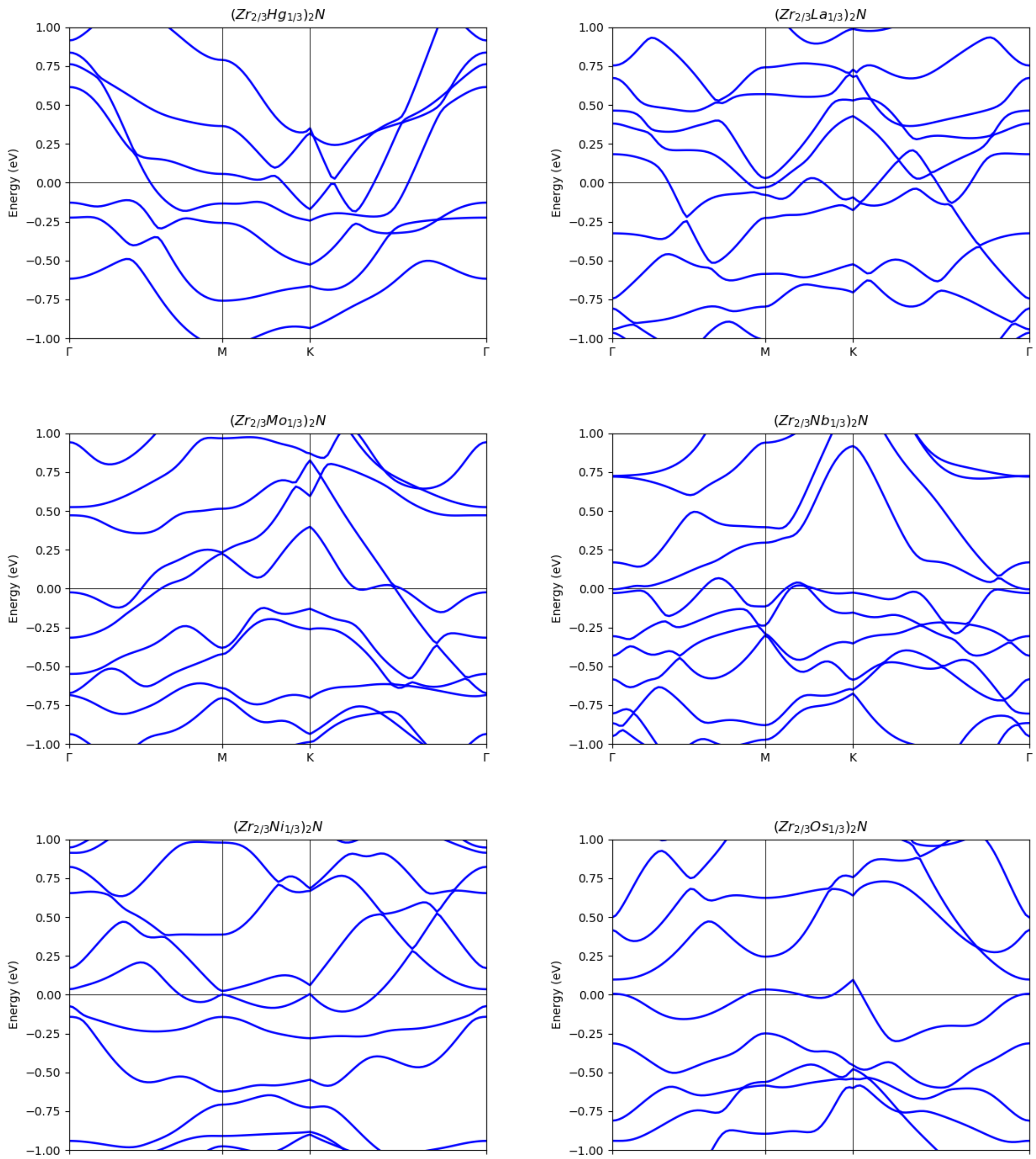

$(Ti_{2/3}Zn_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ

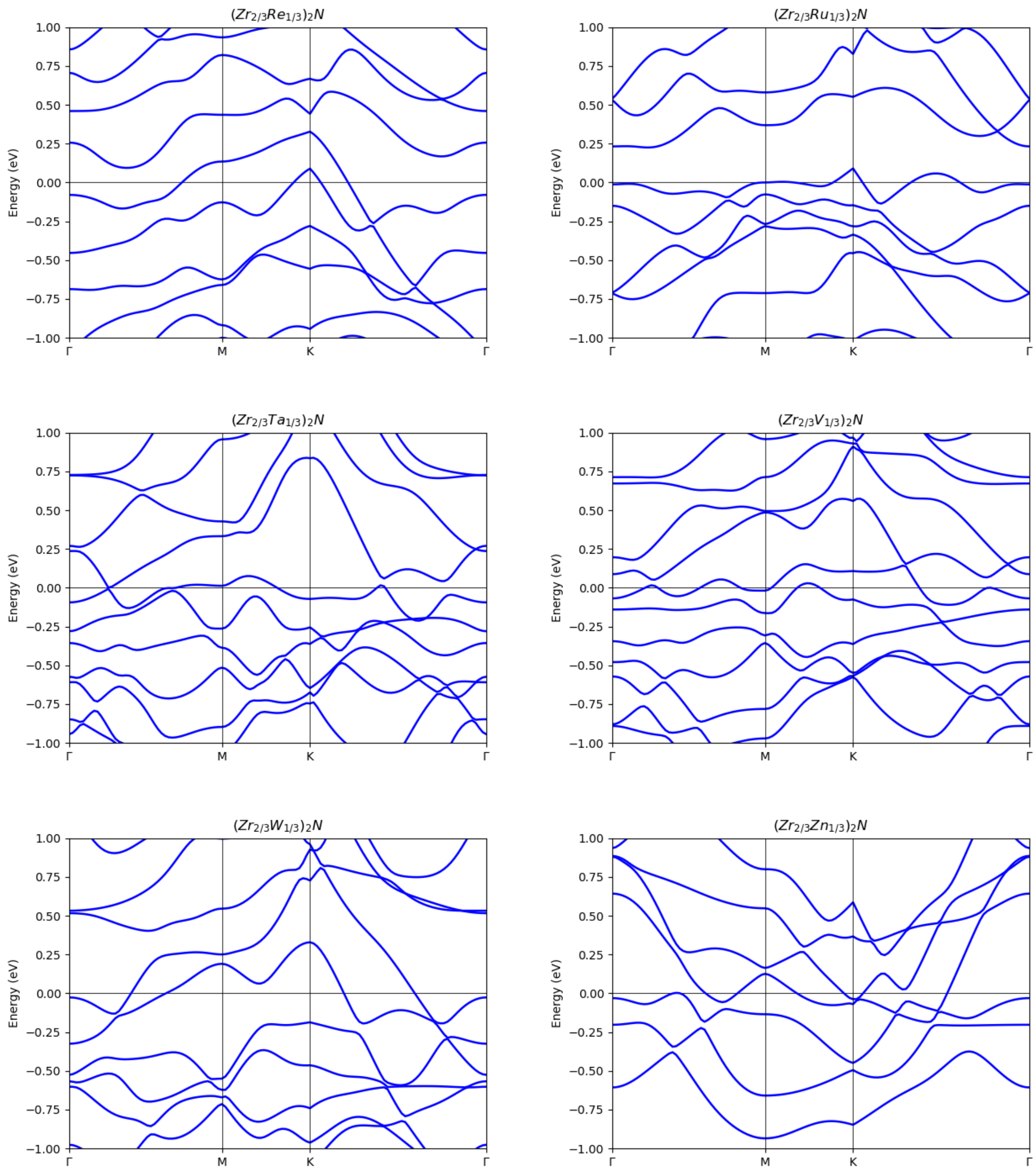

$(Ti_{2/3}Zr_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ


$(Zr_{2/3}Cd_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ


$(Zr_{2/3}Cr_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ


$(Zr_{2/3}Cu_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ


$(Zr_{2/3}Hg_{1/3})_2N$
$(Zr_{2/3}La_{1/3})_2N$
$(Zr_{2/3}Mo_{1/3})_2N$
$(Zr_{2/3}Nb_{1/3})_2N$
$(Zr_{2/3}Ni_{1/3})_2N$
$(Zr_{2/3}Os_{1/3})_2N$
Energy (eV)
Γ
M
K
Γ
1.00
0.75
0.50
0.25
0.00
-0.25
-0.50
-0.75
-1.00


$(Zr_{2/3}Re_{1/3})_2N$
$(Zr_{2/3}Ru_{1/3})_2N$
$(Zr_{2/3}Ta_{1/3})_2N$
$(Zr_{2/3}V_{1/3})_2N$
$(Zr_{2/3}W_{1/3})_2N$
$(Zr_{2/3}Zn_{1/3})_2N$
Energy (eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ