Supplementary Information (SI) for Materials Advances.
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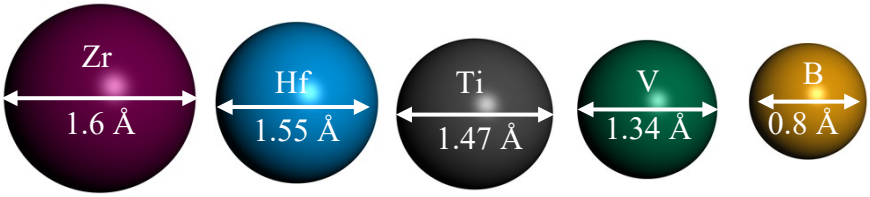
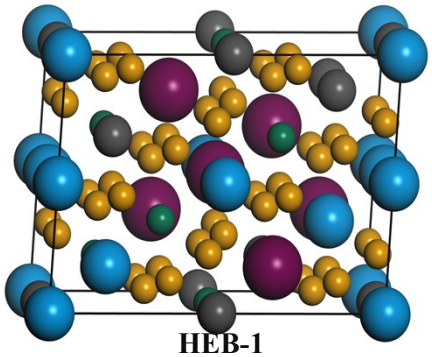
Tailoring the Properties of $(TiZrHfV)B_2$ High-Entropy Diboride via Elemental Concentration: A First-Principles Approach

Nabila Tabassum, Yamini Sudha Sistla*

Supplementary Material

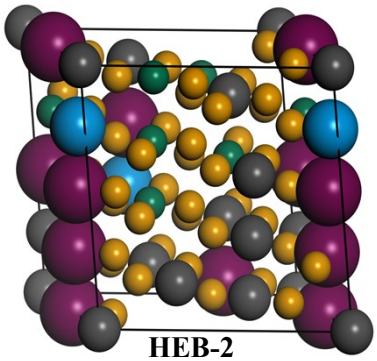
S 1. Optimized crystal structures of HEBs





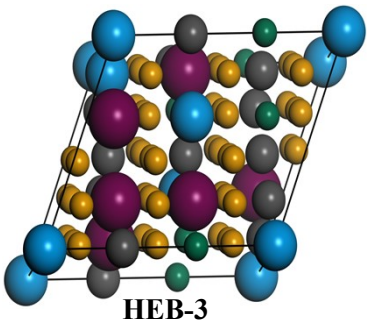
HEB-1

$(Ti_{0.25}Hf_{0.25}Zr_{0.25}V_{0.25})\,B_2$



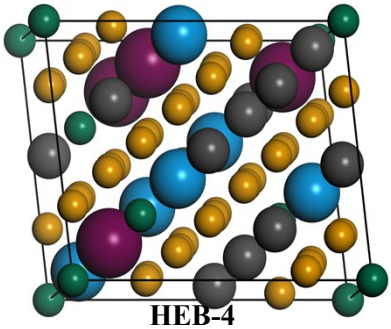
HEB-2

$Ti_{0.42}Hf_{0.08}Zr_{0.25}V_{0.25}B_2$



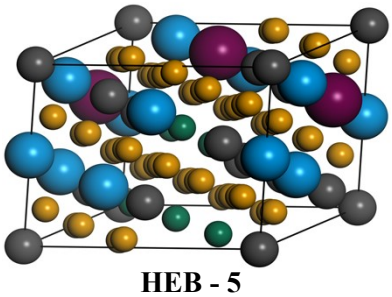
HEB-3

$Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B_2$



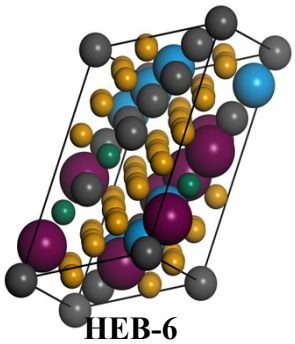
HEB-4

$Ti_{0.42}Hf_{0.25}Zr_{0.17}V_{0.17}B_2$



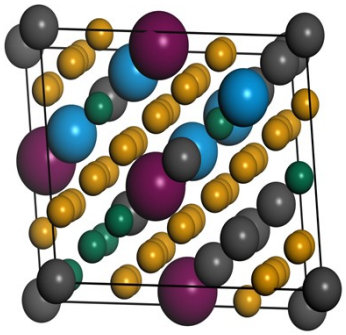
HEB - 5

$Ti_{0.42}Zr_{0.08}(HfV)_{0.25}B_2$



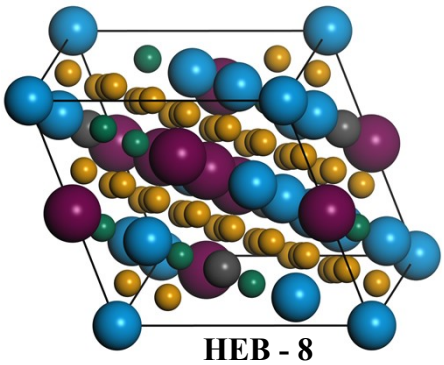
HEB-6

$Ti_{0.42}V_{0.08}(ZrHf)_{0.25}B_2$



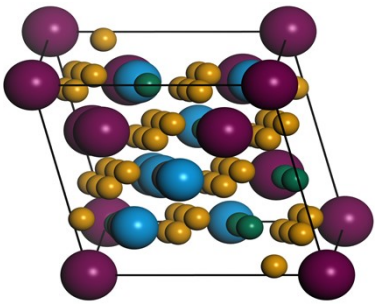
HEB - 7

$Ti_{0.42}V_{0.25}(ZrHf)_{0.17}B_2$



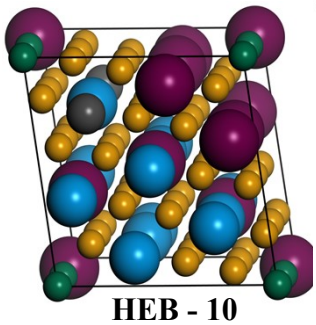
HEB - 8

$Ti_{0.08}Hf_{0.42}(ZrV)_{0.25}B_2$



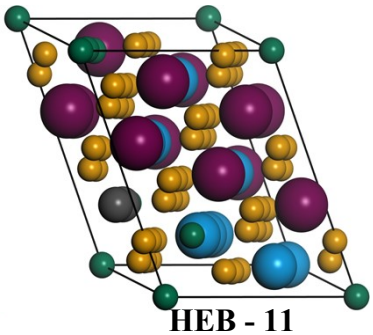
HEB - 9

$Ti_{0.08}V_{0.42}(ZrHf)_{0.25}B_2$



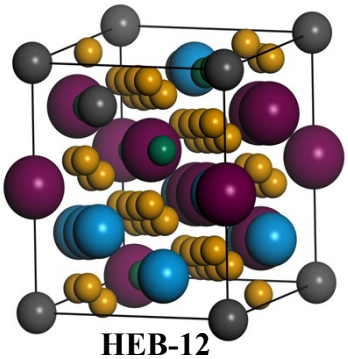
HEB - 10

$Ti_{0.08}V_{0.25}(ZrHf)_{0.33}B_2$



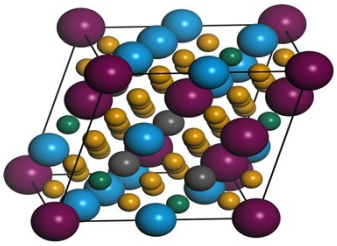
HEB - 11

$Ti_{0.08}Zr_{0.25}(HfV)_{0.33}B_2$



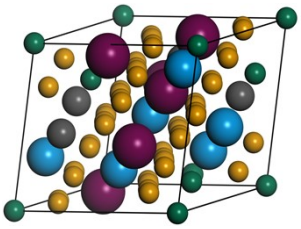
HEB-12

$Ti_{0.08}Hf_{0.25}(ZrV)_{0.3}B_2$



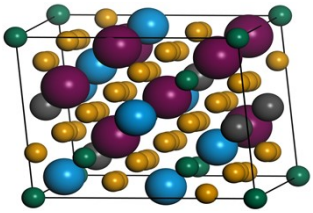
HEB - 13

$Ti_{0.17}Hf_{0.33}(ZrV)_{0.25}B$



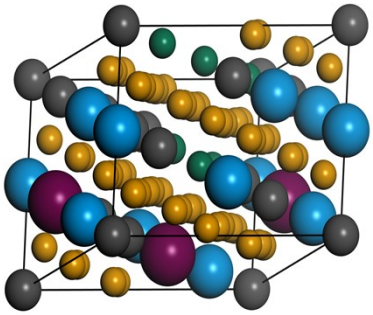
HEB - 14

$Ti_{0.17}V_{0.33}(ZrHf)_{0.25}B_2$



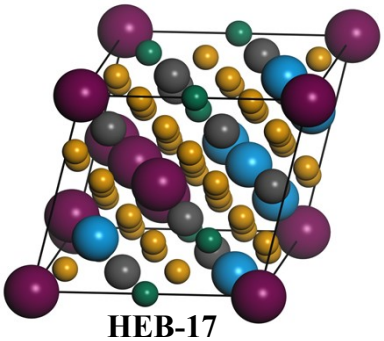
HEB-15

$Ti_{0.17}Zr_{0.33}(HfV)_{0.25}B_2$



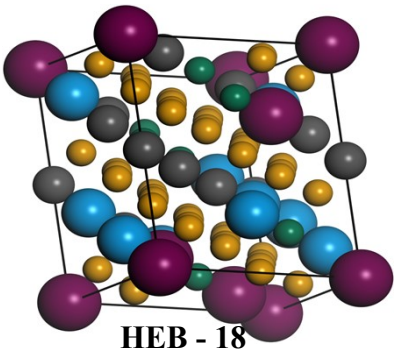
HEB-16

$Ti_{0.33}Hf_{0.17}(ZrV)_{0.25}B_2$



HEB-17

$Ti_{0.33}V_{0.17}(ZrHf)_{0.25}B_2$



HEB - 18

$Ti_{0.33}Zr_{0.17}(HfV)_{0.25}B_2$

Table 1S. Elastic Stiffness Matrix of HEBs Compositions

Elastic Stiffness Matrix of HEB-1 $Ti_{0.25}Zr_{0.25}Hf_{0.25}V_{0.25}B_2$

556.73010	94.76918	64.57952	-18.95585	7.03240	0.96530
94.76918	420.39065	83.95105	56.06512	-1.68843	8.58305
64.57952	83.95105	512.74995	23.71075	0.98542	-2.18970
-18.95585	56.06512	23.71075	187.43625	3.75173	-5.98627
7.03240	-1.68843	0.98542	3.75173	232.58915	19.76888
0.96530	8.58305	-2.18970	-5.98627	19.76888	218.69535

Elastic Stiffness Matrix of HEB-2 $Ti_{0.42}Zr_{0.25}Hf_{0.08}V_{0.25}B_2$

557.66860	84.32350	77.49202	10.62817	4.58682	21.37685
84.32350	465.65750	78.46952	-35.35498	5.03257	38.86912
77.49202	78.46952	568.85335	-18.38748	9.22737	-8.79690
10.62817	-35.35498	-18.38748	209.49205	18.17192	14.98347
4.58682	5.03257	9.22737	18.17192	244.39960	-18.53375
21.37685	38.86912	-8.79690	14.98347	-18.53375	210.20650

Elastic Stiffness Matrix of HEB – 3 $Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B_2$

395.09865	107.33282	99.90845	1.30212	1.58060	-5.08320
107.33282	575.90755	65.62825	-4.18423	-1.56265	2.38890
99.90845	65.62825	572.69825	0.31182	-3.21023	-1.86418
1.30212	-4.18423	0.31182	257.13920	-2.17433	-0.92395
1.58060	-1.56265	-3.21023	-2.17433	232.05190	-3.17850
-5.08320	2.38890	-1.86418	-0.92395	-3.17850	218.53865

Elastic Stiffness Matrix of HEB – 4 $Ti_{0.42}Zr_{0.17}Hf_{0.25}V_{0.17}B_2$

572.50975	84.10615	73.27365	-7.51578	-6.32955	4.85642
84.10615	532.07540	72.00245	33.53967	-10.00598	12.97077
73.27365	72.00245	544.00370	38.36005	-6.99473	5.76902
-7.51578	33.53967	38.36005	204.32300	9.01498	-18.18430
-6.32955	-10.00598	-6.99473	9.01498	237.01965	16.69183
4.85642	12.97077	5.76902	-18.18430	16.69183	248.10825

Elastic Stiffness Matrix of HEB – 5 $Ti_{0.42}Zr_{0.08}Hf_{0.25}V_{0.25}B_2$

576.02840	76.52787	85.72152	3.14812	-10.94648	24.74930
76.52787	511.34005	88.48008	24.43950	-8.60465	48.46077
85.72152	88.48008	605.64050	6.15990	-13.52150	-12.55242
3.14812	24.43950	6.15990	226.47210	24.44458	-22.41320

-10.94648 -8.60465 -13.52150 24.44458 256.87855 16.69590
24.74930 48.46077 -12.55242 -22.41320 16.69590 206.2656

Elastic Stiffness Matrix of HEB – 6 $Ti_{0.42}Zr_{0.25}Hf_{0.25}V_{0.08}B_2$

569.78985 70.82425 86.59593 -8.23865 5.32390 28.99487
70.82425 539.08805 106.82252 -5.27685 8.55492 28.03510
86.59593 106.82252 576.20345 -13.68095 1.14785 -10.32463
-8.23865 -5.27685 -13.68095 248.24590 15.65032 26.38250
5.32390 8.55492 1.14785 15.65032 255.24390 -17.05457
28.99487 28.03510 -10.32463 26.38250 -17.05457 212.26245

Elastic Stiffness Matrix of HEB – 7 $Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B_2$

589.52175 83.00212 80.56850 -5.99030 -6.97918 6.14145
83.00212 535.67120 86.31212 41.36855 -4.66110 16.88107
80.56850 86.31212 552.32635 33.23707 -12.30785 7.70350
-5.99030 41.36855 33.23707 207.14195 10.46945 -17.15182
-6.97918 -4.66110 -12.30785 10.46945 239.35265 19.72975
6.14145 16.88107 7.70350 -17.15182 19.72975 241.80205

Elastic Stiffness Matrix of HEB – 8 $Ti_{0.08}Zr_{0.25}Hf_{0.42}V_{0.25}B_2$

571.32870 109.59583 89.14262 12.85165 -7.73948 -2.48430
109.59583 466.40560 103.19507 -47.61845 -5.35143 -41.68485
89.14262 103.19507 575.16140 -4.50110 1.14190 8.33082
12.85165 -47.61845 -4.50110 204.21110 -12.31523 -22.73065
-7.73948 -5.35143 1.14190 -12.31523 241.67585 -15.11855
-2.48430 -41.68485 8.33082 -22.73065 -15.11855 211.78420

Elastic Stiffness Matrix of HEB – 9 $Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B_2$

553.94970 80.32500 92.26710 -15.39128 -10.05208 7.79600
80.32500 485.52050 98.23570 48.53663 -1.16930 29.31372
92.26710 98.23570 476.43920 40.26717 -12.81543 3.96252
-15.39128 48.53663 40.26717 182.60070 12.11595 -16.50077
-10.05208 -1.16930 -12.81543 12.11595 213.64435 22.82308
7.79600 29.31372 3.96252 -16.50077 22.82308 221.81825

Elastic Stiffness Matrix of HEB – 10 $Ti_{0.08}Zr_{0.33}Hf_{0.33}V_{0.25}B_2$

362.82115 123.17542 106.59197 9.10832 -2.14823 0.36360
123.17542 553.35200 53.82307 -2.26595 1.54510 4.16042
106.59197 53.82307 562.17545 -0.29020 1.00355 0.18040
9.10832 -2.26595 -0.29020 252.60605 0.77153 -0.71152

-2.14823	1.54510	1.00355	0.77153	215.05375	-4.90680
0.36360	4.16042	0.18040	-0.71152	-4.90680	213.66880

Elastic Stiffness Matrix of HEB – 11 $Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B_2$

467.58330	79.80223	87.30005	-4.59910	43.04692	-25.29508
79.80223	540.31055	82.76798	2.50850	-13.11825	-2.44885
87.30005	82.76798	496.14070	23.26842	33.93590	3.42392
-4.59910	2.50850	23.26842	217.18745	-14.00335	19.32183
43.04692	-13.11825	33.93590	-14.00335	184.99240	14.35162
-25.29508	-2.44885	3.42392	19.32183	14.35162	208.70090

Elastic Stiffness Matrix of HEB – 12 $Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B_2$

547.23280	83.77102	81.36687	2.53177	25.44882	11.45492
83.77102	560.44530	84.82408	-10.67760	-8.81205	8.01735
81.36687	84.82408	501.06355	-32.27535	37.53530	5.62170
2.53177	-10.67760	-32.27535	207.68830	24.68105	21.28740
25.44882	-8.81205	37.53530	24.68105	193.92280	-21.87167
11.45492	8.01735	5.62170	21.28740	-21.87167	230.44595

Elastic Stiffness Matrix of HEB – 13 ($Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B$)

537.82250	101.42677	85.25675	-1.14600	37.86535	3.93957
101.42677	571.07480	97.04162	-0.51515	-17.23470	4.40348
85.25675	97.04162	522.27650	-20.43298	41.05105	6.73597
-1.14600	-0.51515	-20.43298	229.76560	18.37783	18.84150
37.86535	-17.23470	41.05105	18.37783	182.95820	-12.80665
3.93957	4.40348	6.73597	18.84150	-12.80665	242.18260

Elastic Stiffness Matrix of HEB – 14 $Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B_2$

539.60185	88.65400	83.43545	-0.19723	-23.57785	27.06627
88.65400	532.60925	89.10010	29.48322	4.31877	23.14602
83.43545	89.10010	520.92235	28.89537	-22.58273	-2.74870
-0.19723	29.48322	28.89537	190.99165	25.00425	-24.70265
-23.57785	4.31877	-22.58273	25.00425	209.23360	28.02603
27.06627	23.14602	-2.74870	-24.70265	28.02603	211.73150

Elastic Stiffness Matrix of HEB – 15 $Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B_2$

563.29415	102.72135	85.33273	-10.82603	1.58240	6.38740
102.72135	501.70630	74.56733	36.83750	-1.81498	-3.96750
85.33273	74.56733	542.27780	37.13712	-8.07965	-0.27903
-10.82603	36.83750	37.13712	189.77870	-1.35582	-10.33822

1.58240	-1.81498	-8.07965	-1.35582	226.43030	12.87295
6.38740	-3.96750	-0.27903	-10.33822	12.87295	238.50375

Elastic Stiffness Matrix of HEB – 16 $Ti_{0.33}Zr_{0.25}Hf_{0.17}V_{0.25}B_2$

468.65590	90.40512	91.29852	7.27140	-39.51085	39.44737
90.40512	576.35020	76.00615	4.14102	8.65962	13.49837
91.29852	76.00615	573.43790	6.35937	-13.16955	-9.20032
7.27140	4.14102	6.35937	248.14090	15.85870	-15.70337
-39.51085	8.65962	-13.16955	15.85870	215.10370	16.62148
39.44737	13.49837	-9.20032	-15.70337	16.62148	212.97485

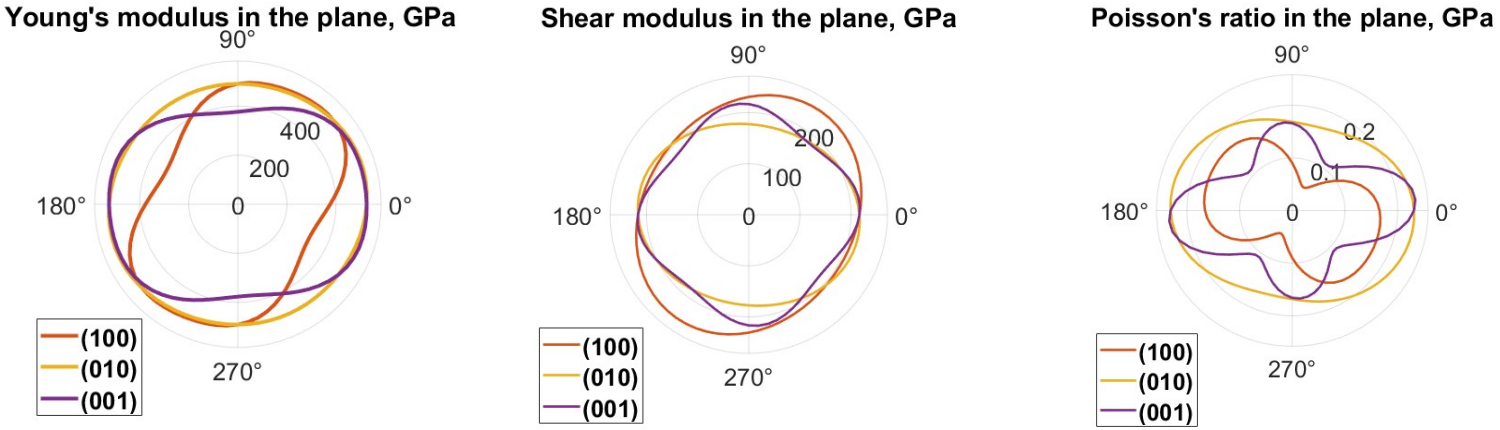
Elastic Stiffness Matrix of HEB – 17 $Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B_2$

559.48155	81.78723	79.77320	3.48107	20.17102	-31.34403
81.78723	561.53950	86.60227	17.74230	4.29137	-26.26570
79.77320	86.60227	595.68225	9.00087	10.39120	12.06605
3.48107	17.74230	9.00087	238.86350	-16.64142	28.11625
20.17102	4.29137	10.39120	-16.64142	236.17810	24.23778
-31.34403	-26.26570	12.06605	28.11625	24.23778	209.68495

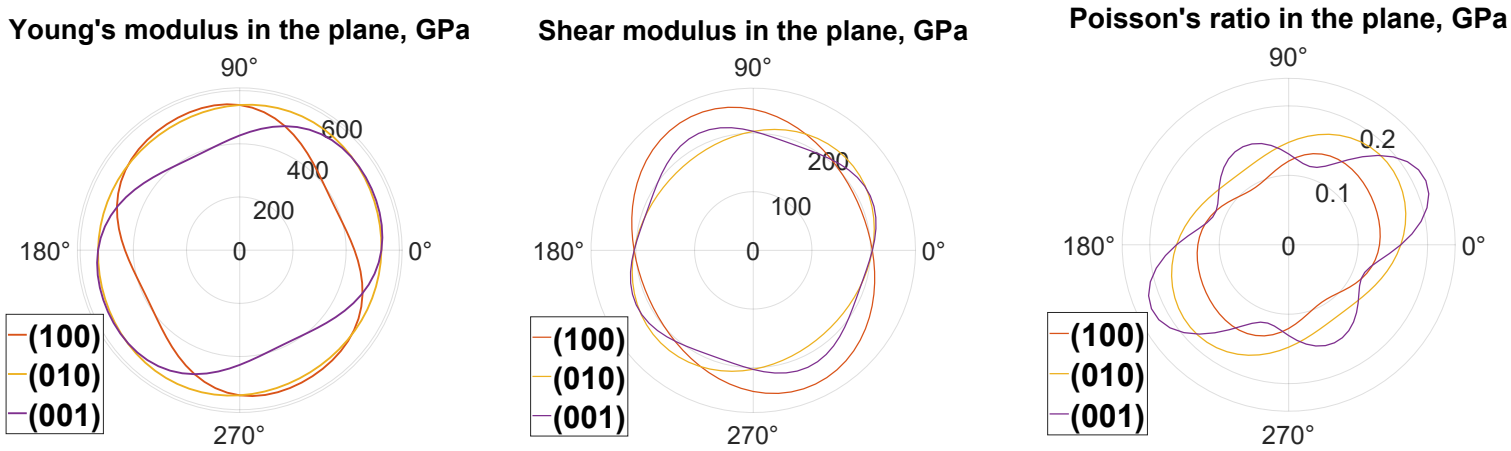
Elastic Stiffness Matrix of HEB – 18 $Ti_{0.33}Zr_{0.17}Hf_{0.25}V_{0.25}B_2$

566.10345	85.54028	92.62707	-0.78413	23.25277	7.57020
85.54028	579.35605	83.14775	-16.82805	-9.07100	7.14685
92.62707	83.14775	525.37955	-25.02680	38.09272	11.43040
-0.78413	-16.82805	-25.02680	223.19910	25.47757	18.37398
23.25277	-9.07100	38.09272	25.47757	206.46930	-27.52515
7.57020	7.14685	11.43040	18.37398	-27.52515	231.57425

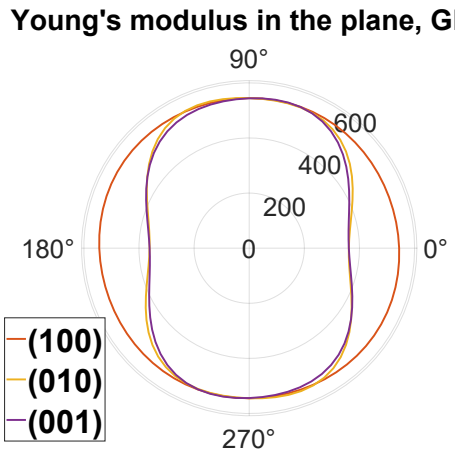
S 2. 2D projected Young's modulus, shear modulus and Poisson's ratio in (100), (010) and (001) planes with respect to rotation angle

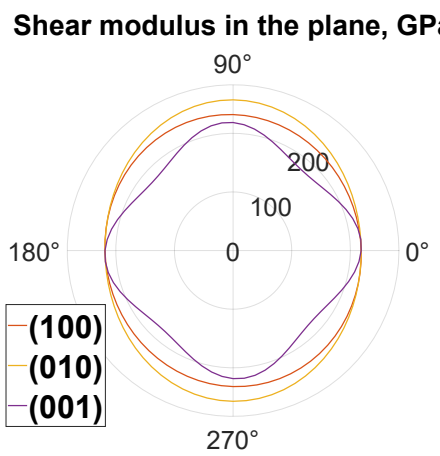


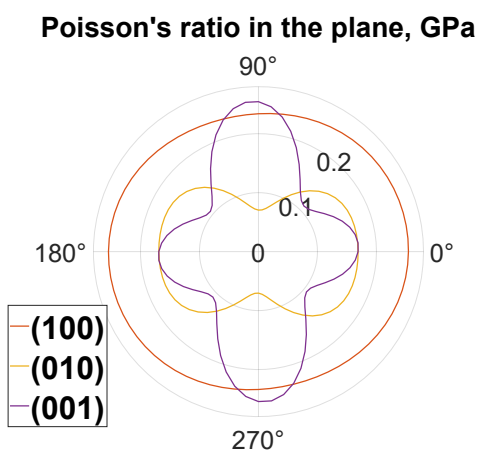
HEB-1 $Ti_{0.25}Zr_{0.25}Hf_{0.25}V_{0.25}B_2$



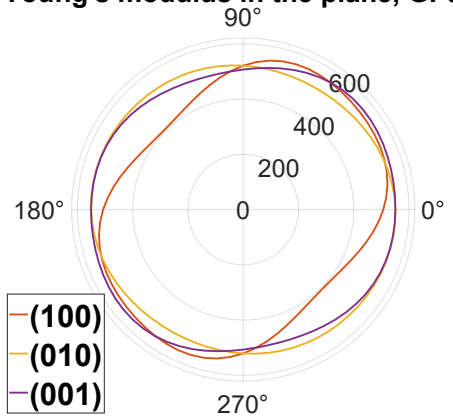
HEB – 2 $Ti_{0.42}Zr_{0.25}Hf_{0.08}V_{0.25}B_2$

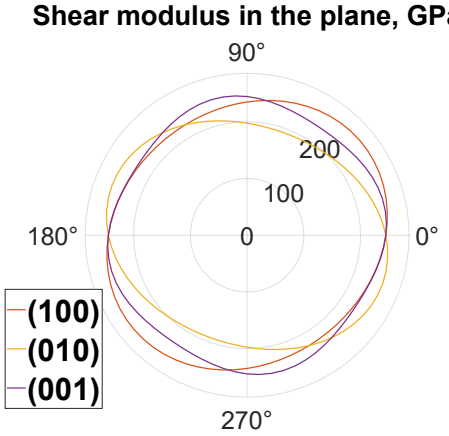


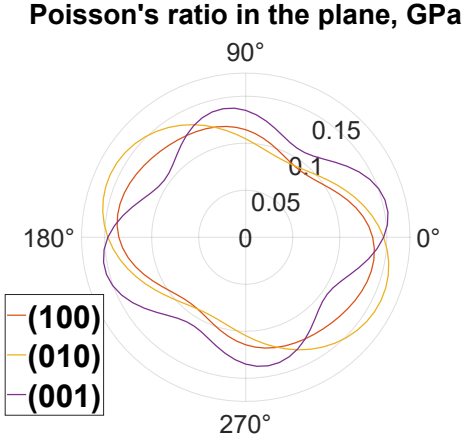




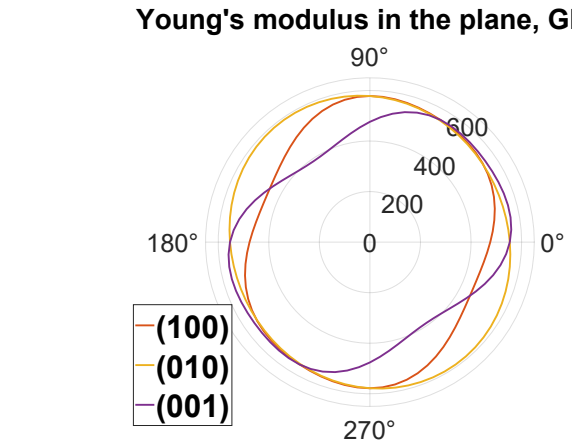
HEB – 3 $Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B_2$

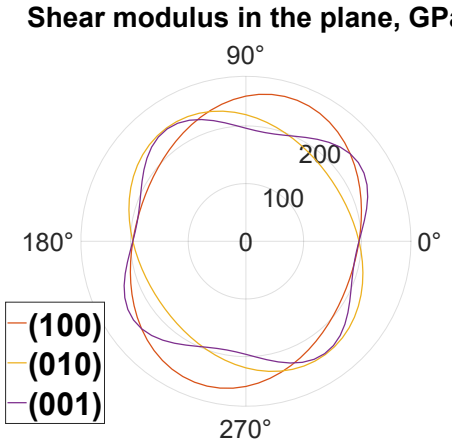


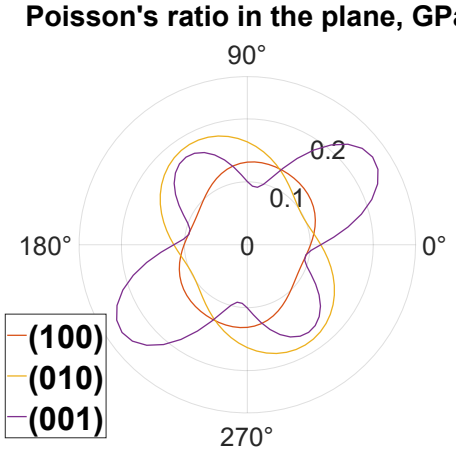




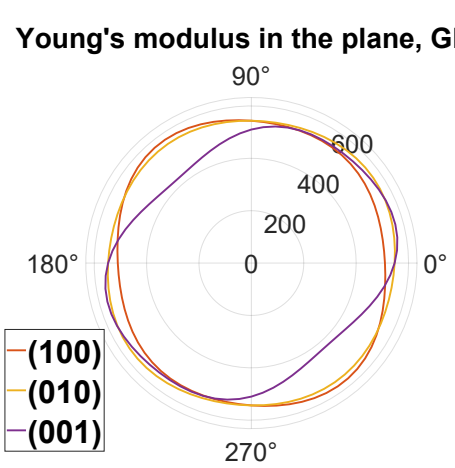
HEB – 4 $Ti_{0.42}Zr_{0.17}Hf_{0.25}V_{0.17}B_2$

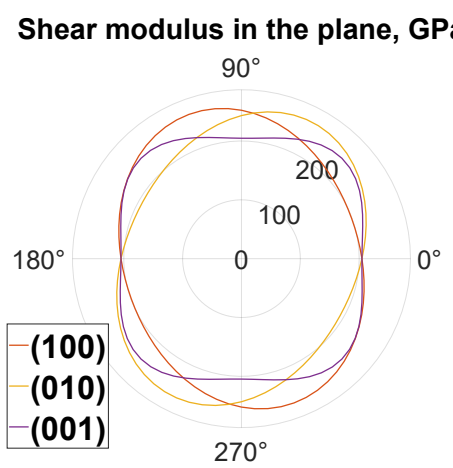


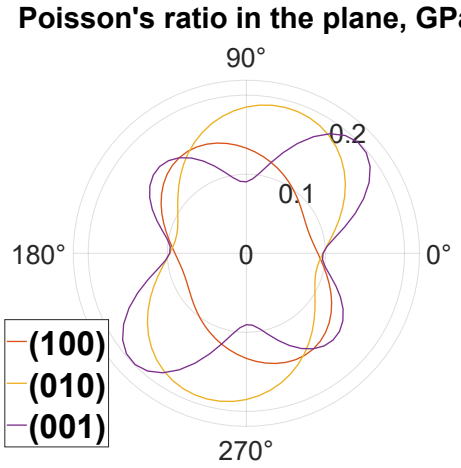




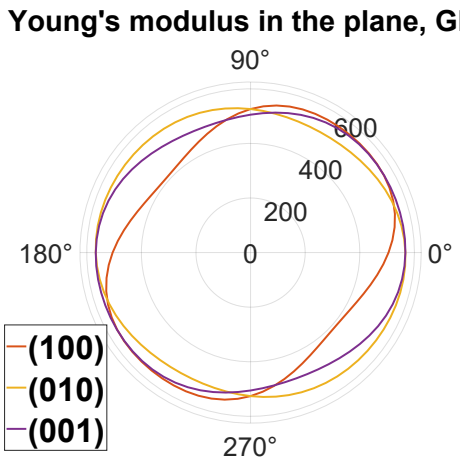
HEB – 5 $Ti_{0.42}Zr_{0.08}Hf_{0.25}V_{0.25}B_2$

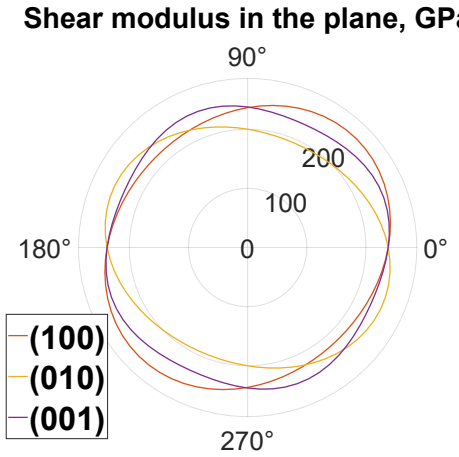


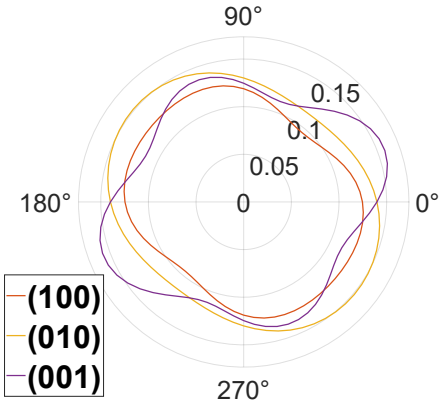




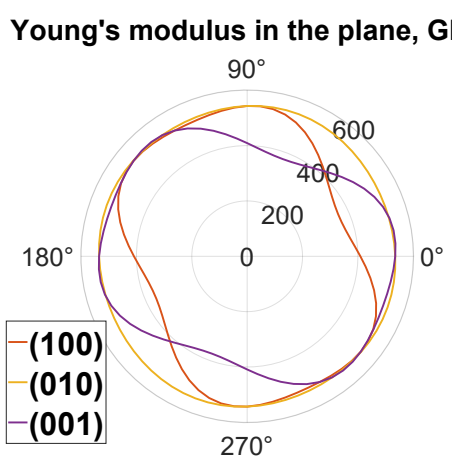
HEB – 6 $Ti_{0.42}Zr_{0.25}Hf_{0.25}V_{0.08}B_2$

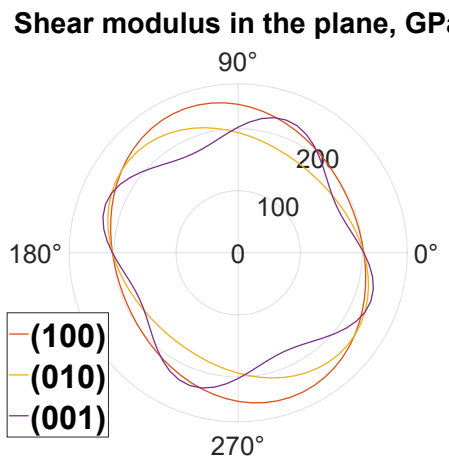


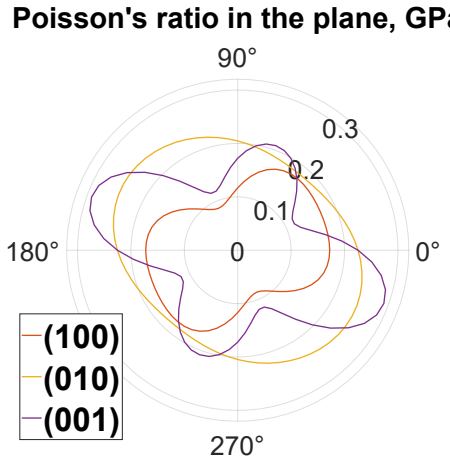




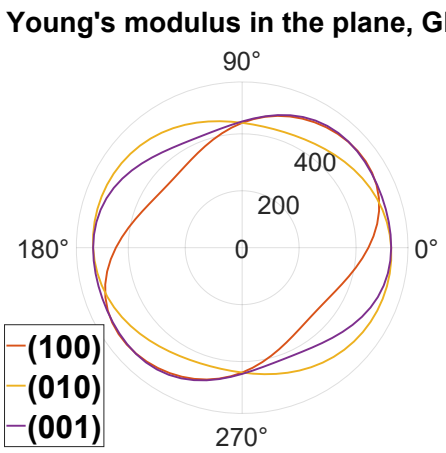
HEB – 7 $Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B_2$

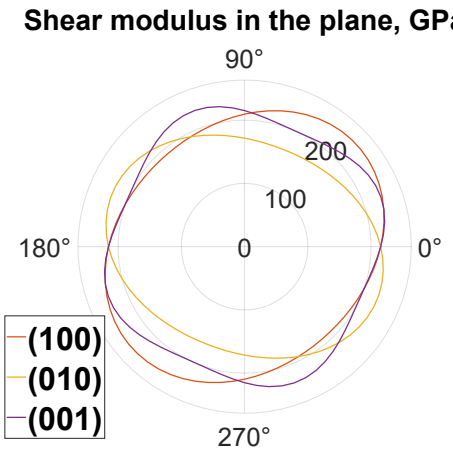


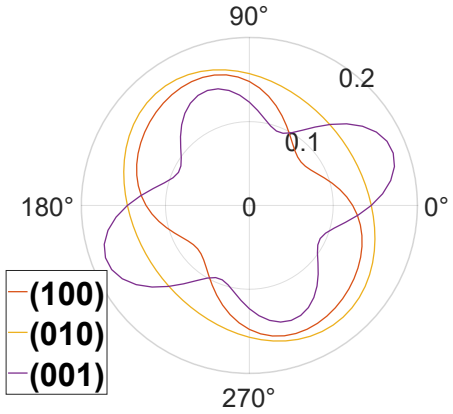




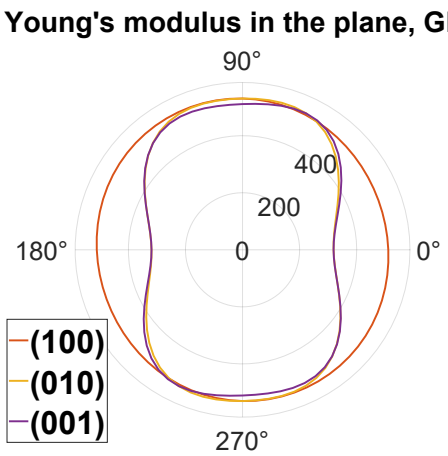
HEB – 8 $Ti_{0.08}Zr_{0.25}Hf_{0.42}V_{0.25}B_2$

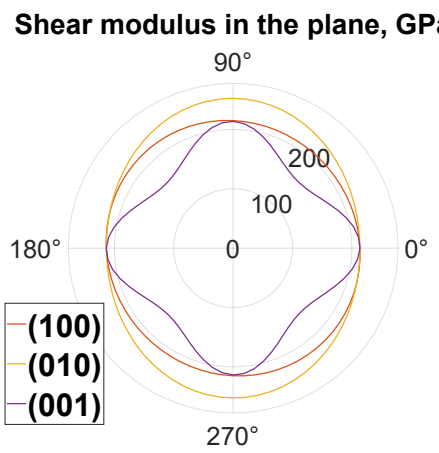


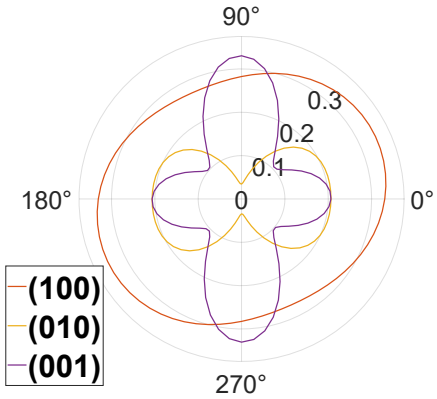




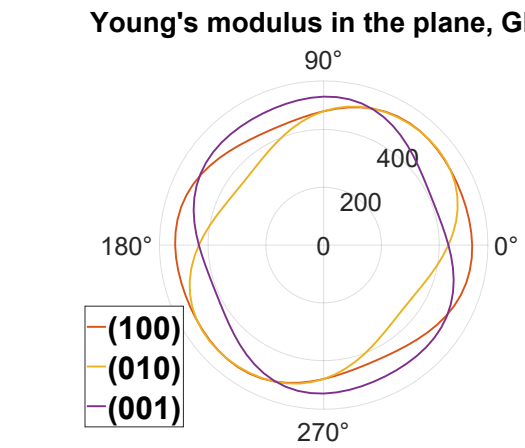
HEB – 9 $Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B_2$

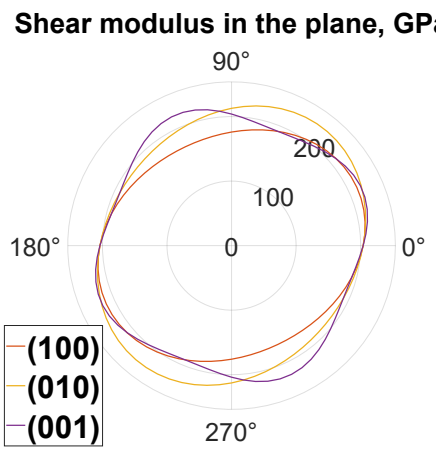


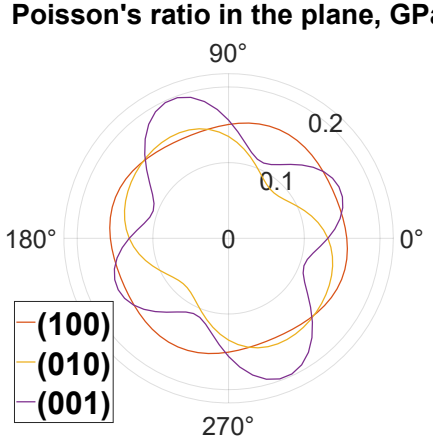




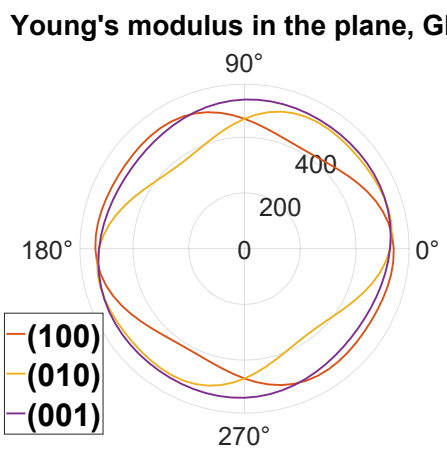
HEB – 10 $Ti_{0.08}Zr_{0.33}Hf_{0.33}V_{0.25}B_2$

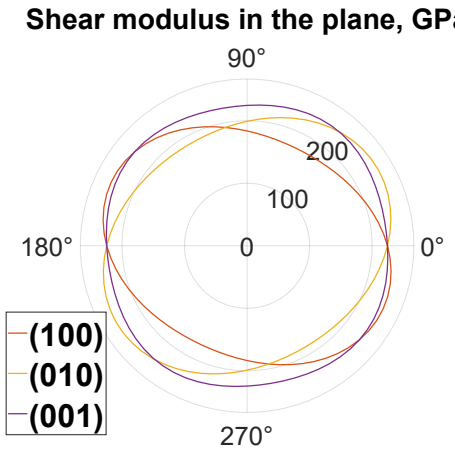


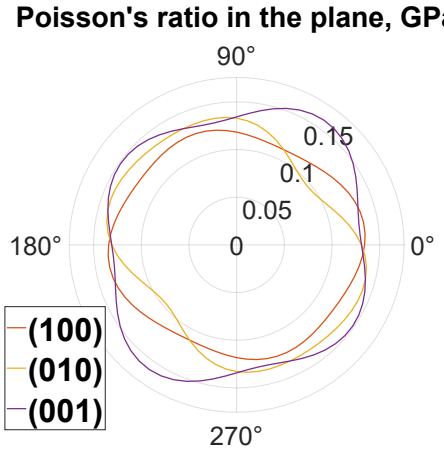




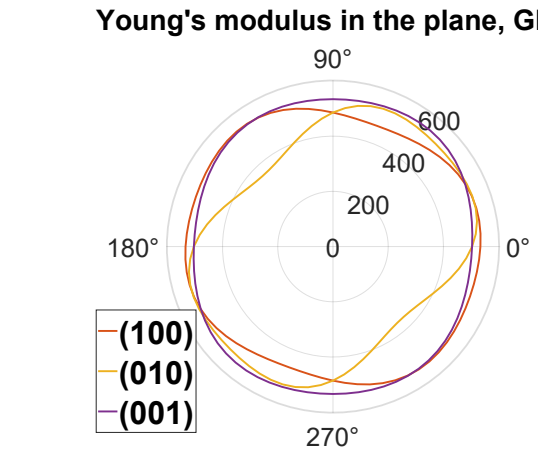
HEB – 11 $Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B_2$

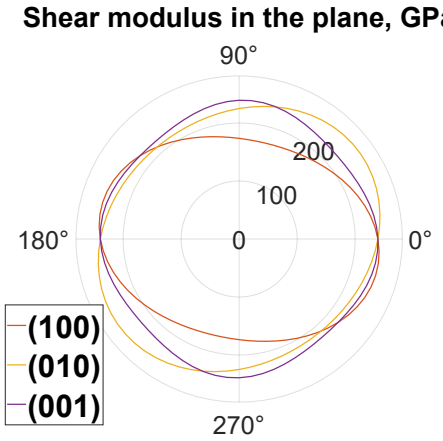


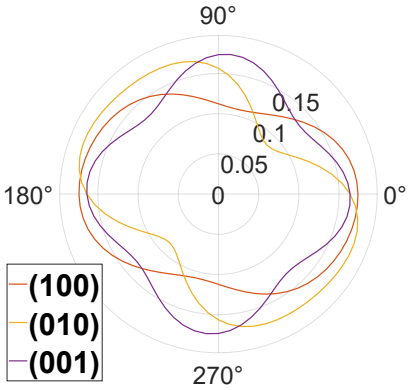




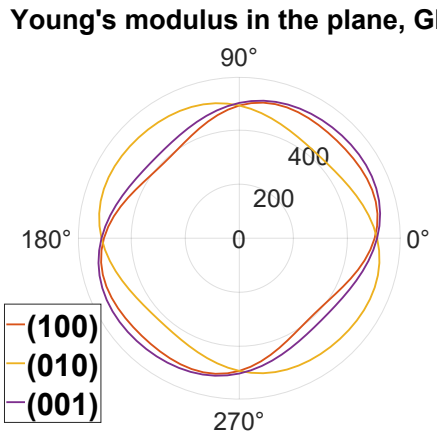
HEB – 12 $Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B_2$

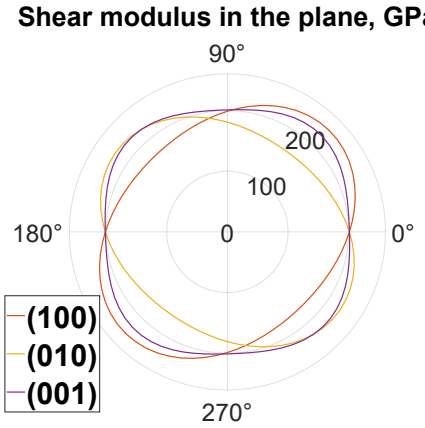


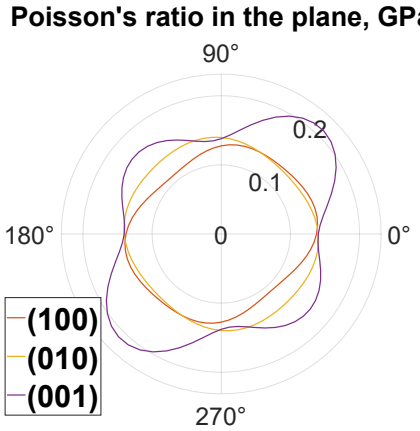




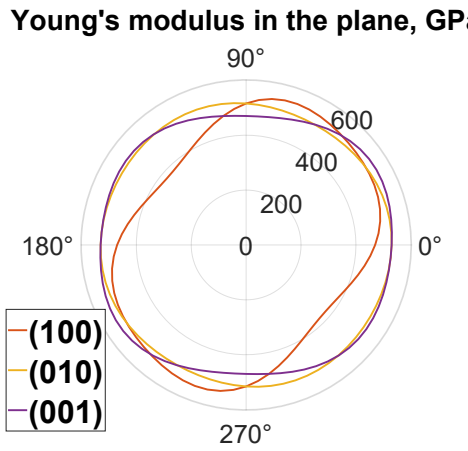
HEB – 13 $Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B_2$

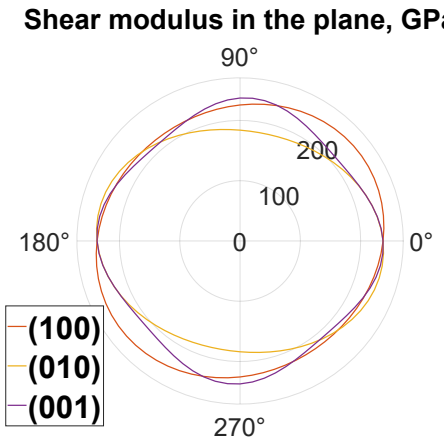


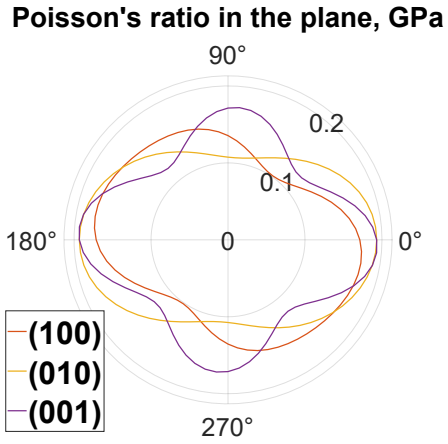




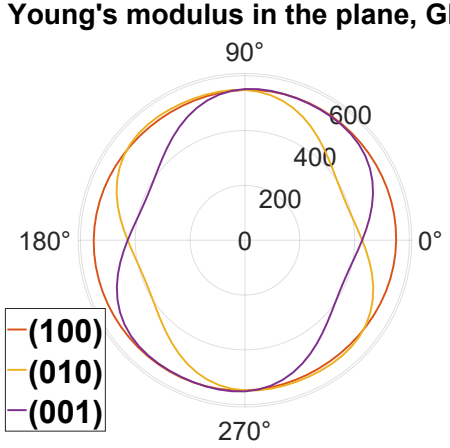
HEB – 14 $Ti_{0.17}Zr_{0.25}Hf_{0.25}V_{0.33}B_2$

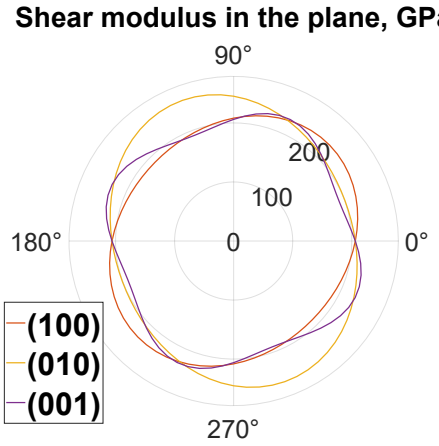


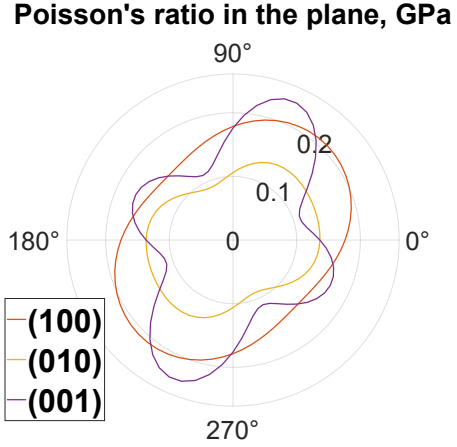




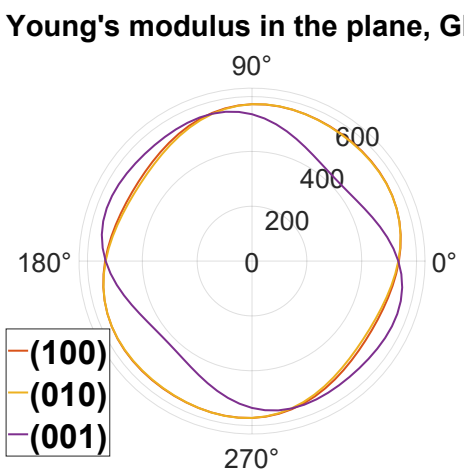
HEB – 15 $Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B_2$

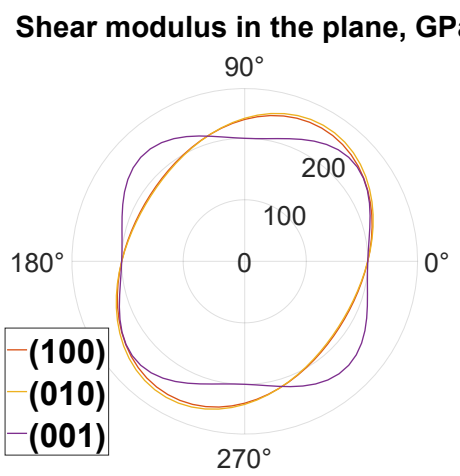


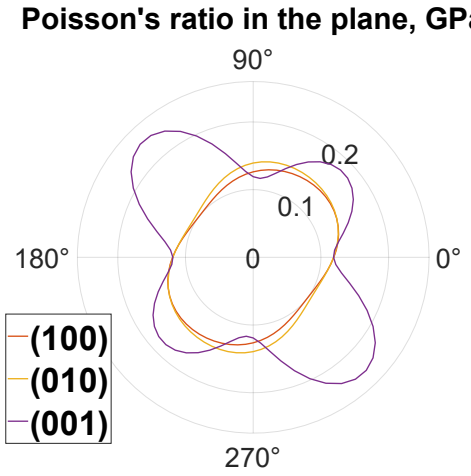




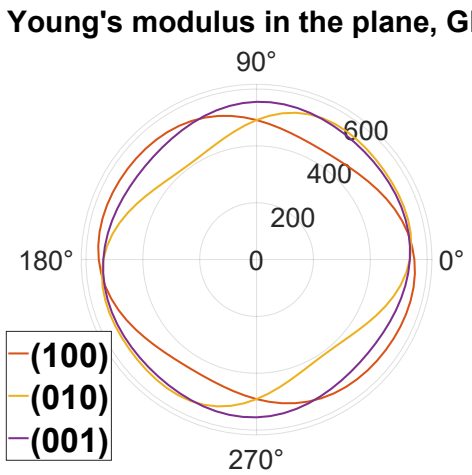
HEB – 16 $Ti_{0.33}Zr_{0.25}Hf_{0.17}V_{0.25}B_2$

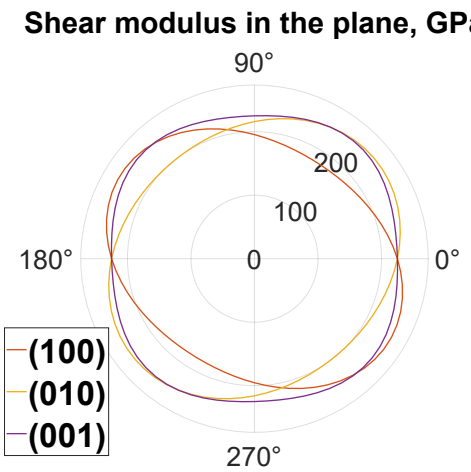


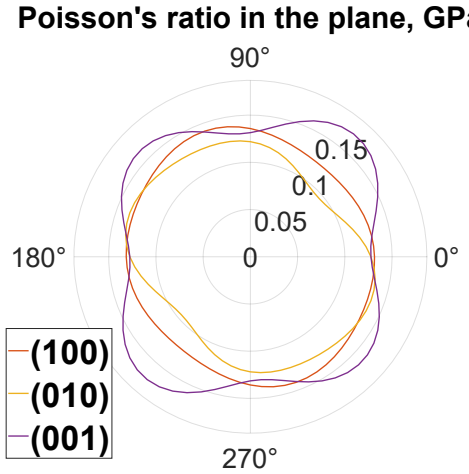




HEB – 17 $Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B_2$



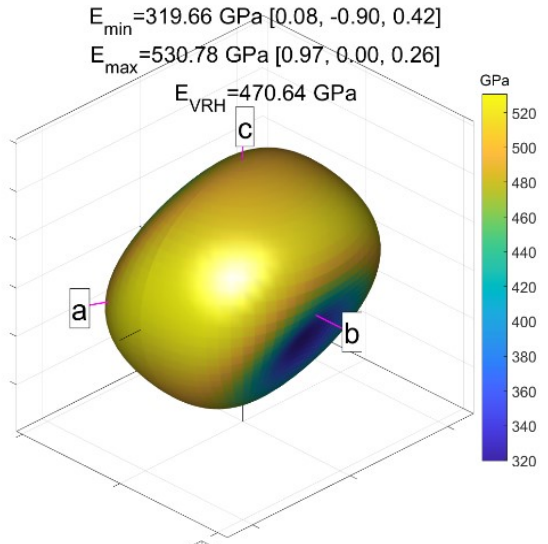


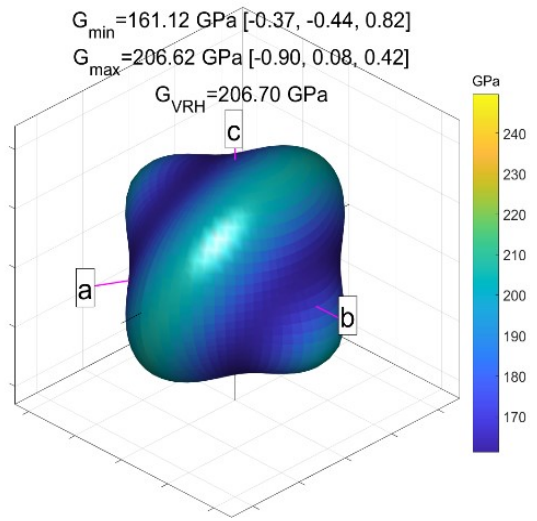


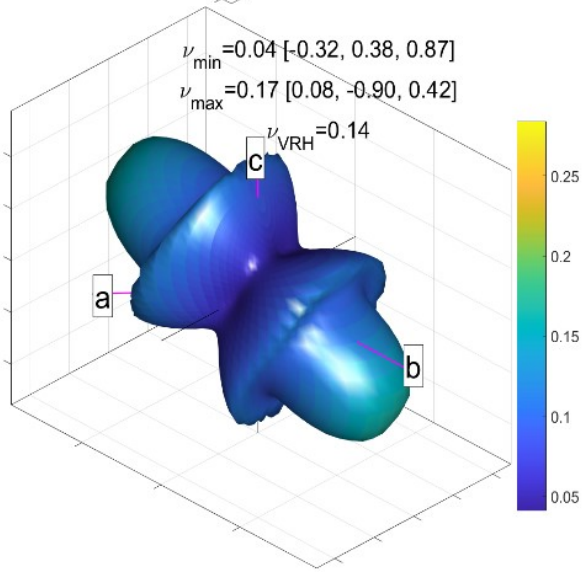
HEB – 18 $Ti_{0.33}Zr_{0.17}Hf_{0.25}V_{0.25}B_2$

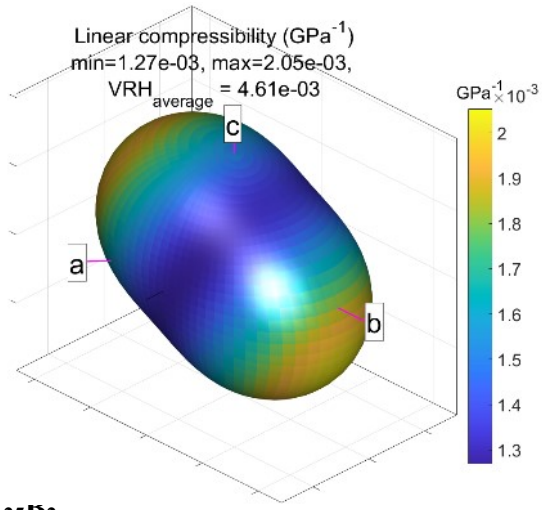
3D projected Young's modulus, Shear modulus, Poisson's ratio, and Compressibility

HEB – 1 $Ti_{0.25}Zr_{0.25}Hf_{0.25}V_{0.25}B_2$

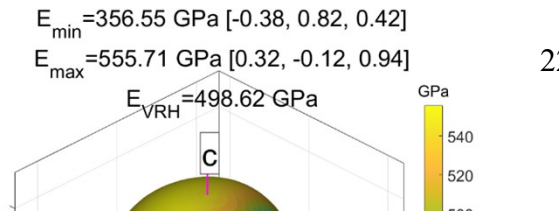


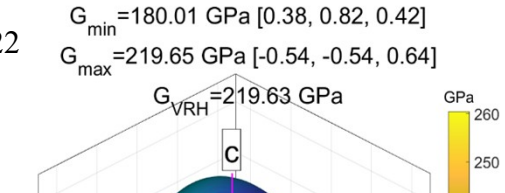


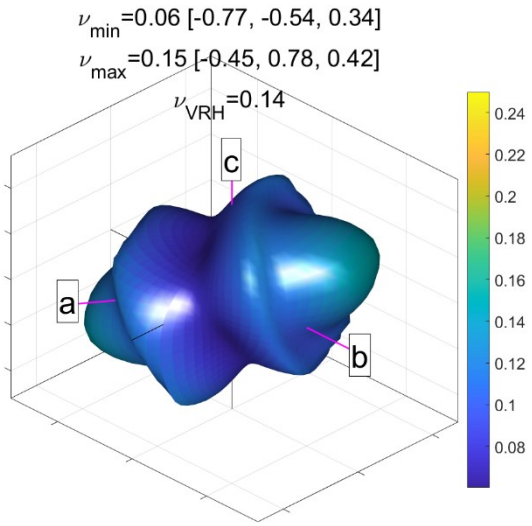


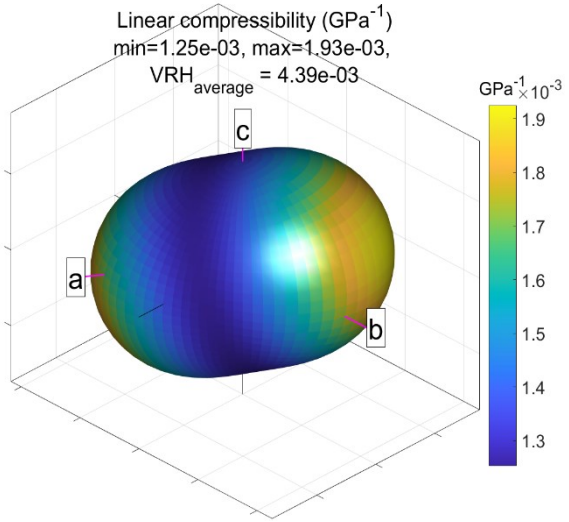


HEB-2 $Ti_{0.42}Zr_{0.25}Hf_{0.08}V_{0.25}B_2$

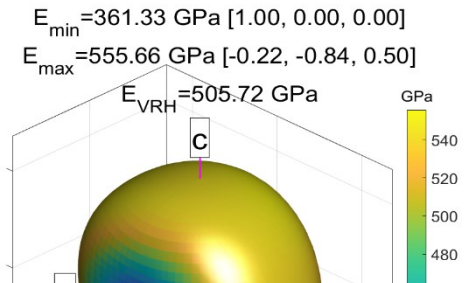


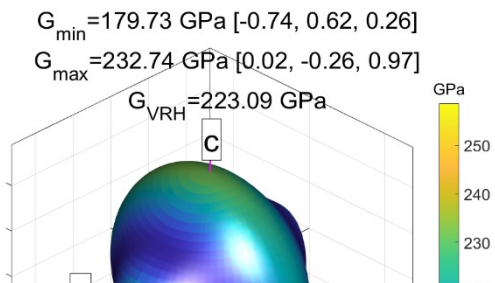


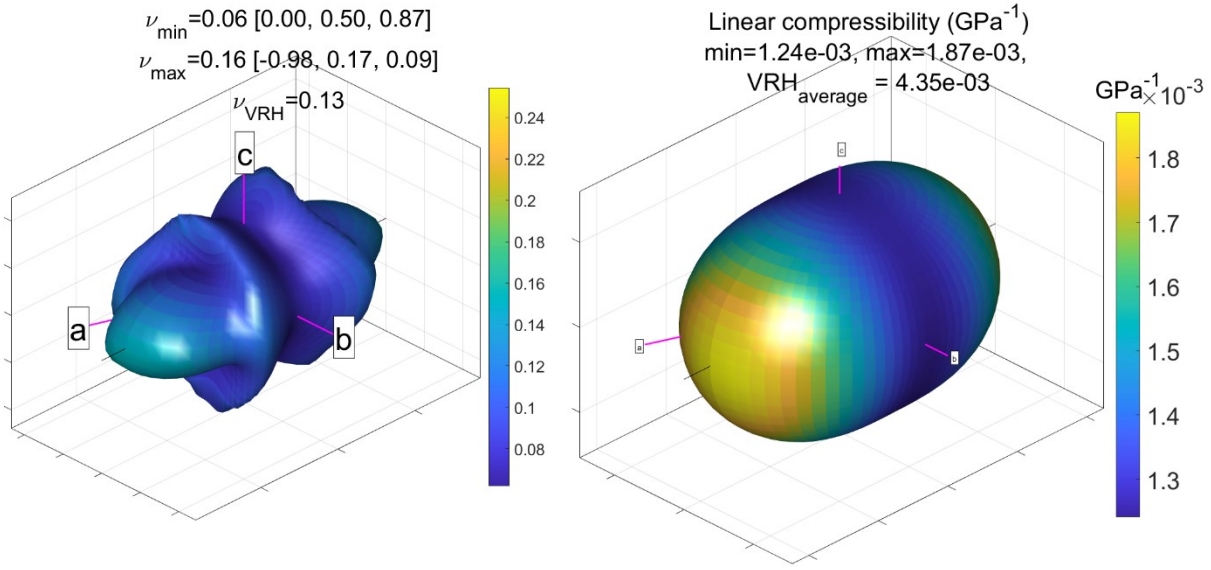




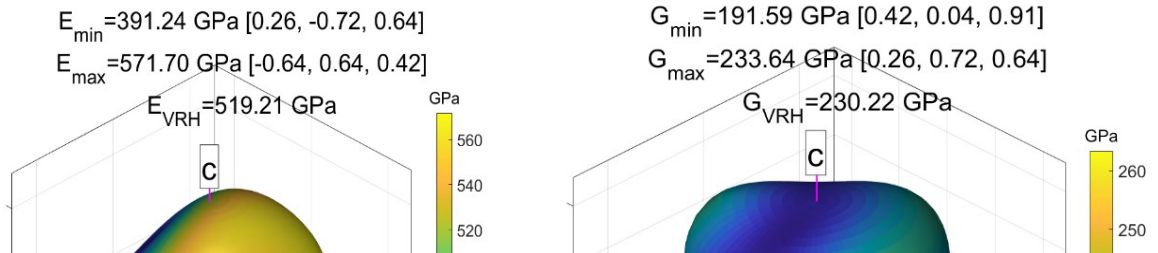
HEB-3 $Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B_2$

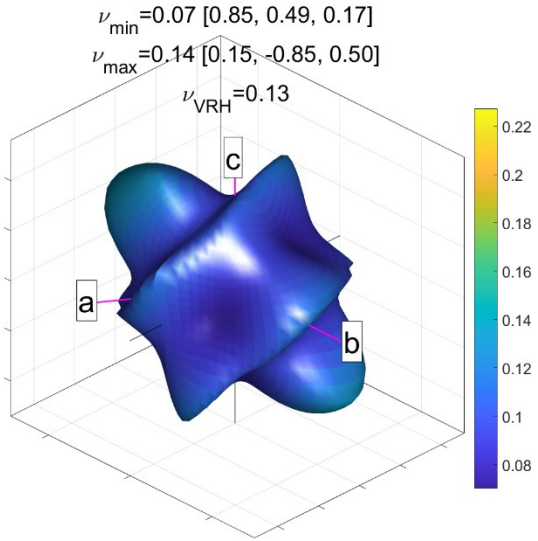


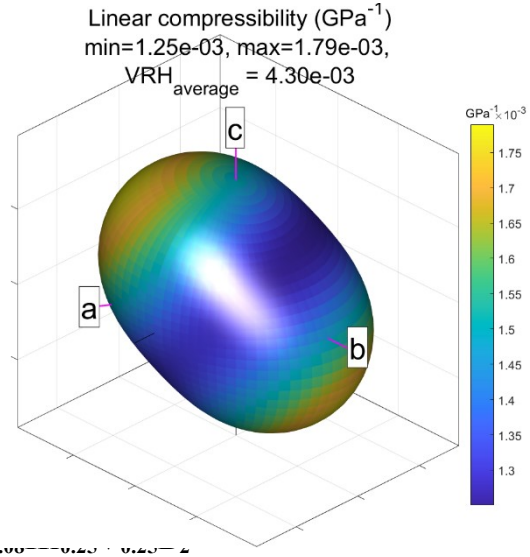




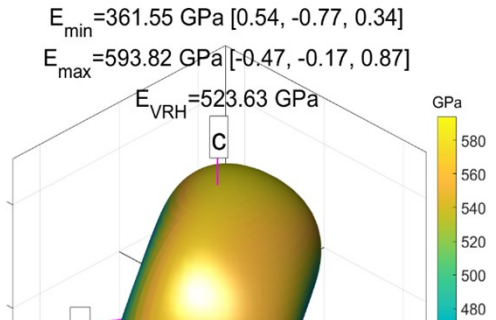
HEB-4 $Ti_{0.42}Zr_{0.17}Hf_{0.25}V_{0.17}B_2$

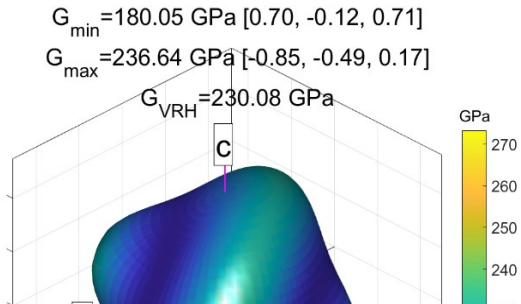


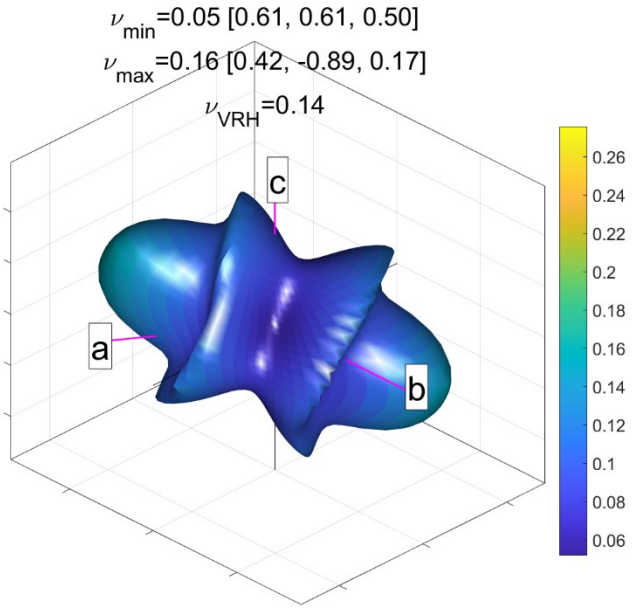


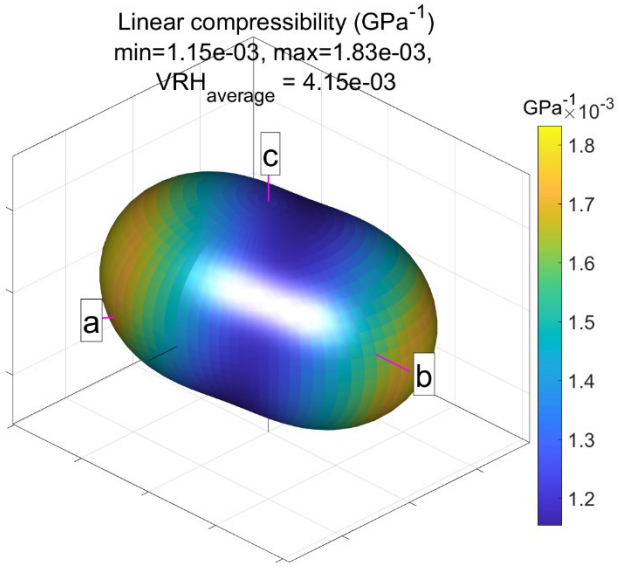


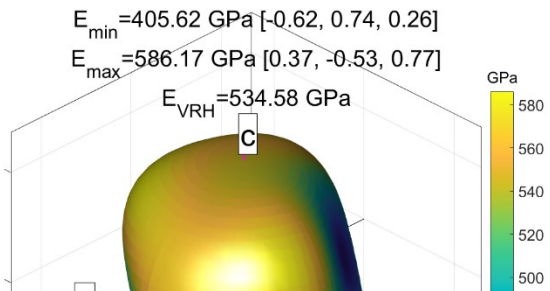
HEB-5 $Ti_{0.42}Zr_{0.}$

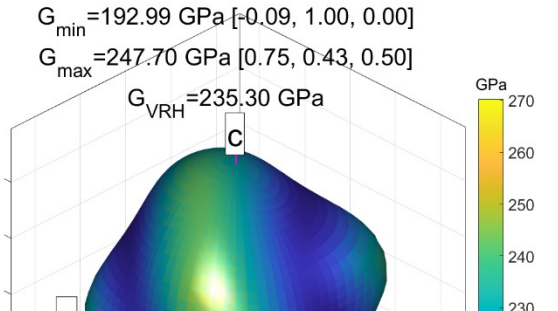


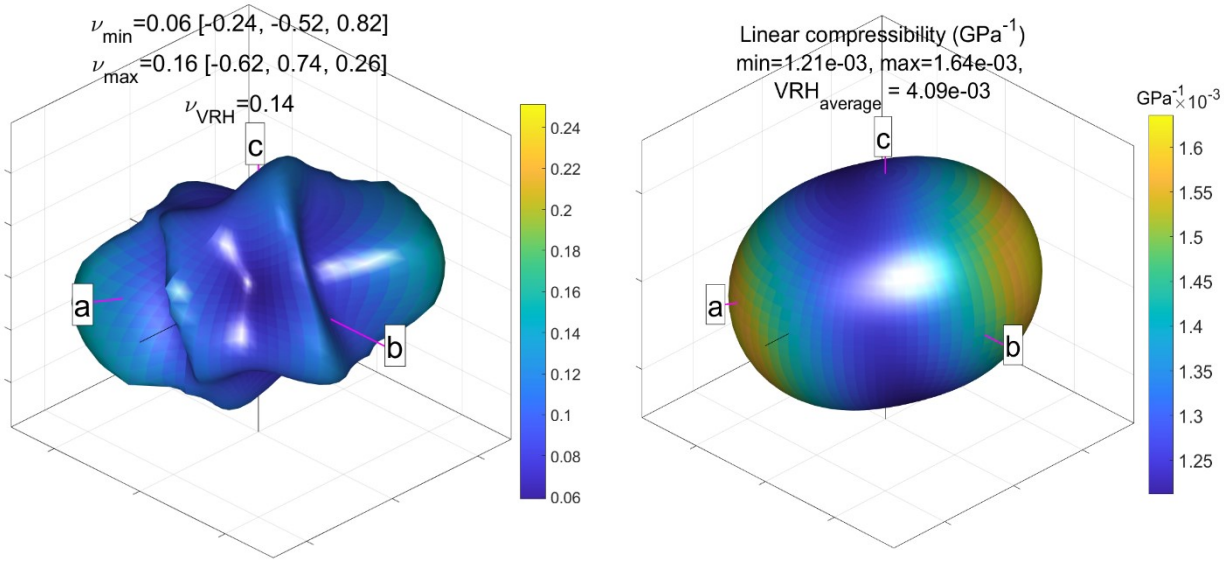



ν_{min}=0.05 [0.61, 0.61, 0.50]
ν_{max}=0.16 [0.42, -0.89, 0.17]
ν_{VRH}=0.14
c
a
b
0.26
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06

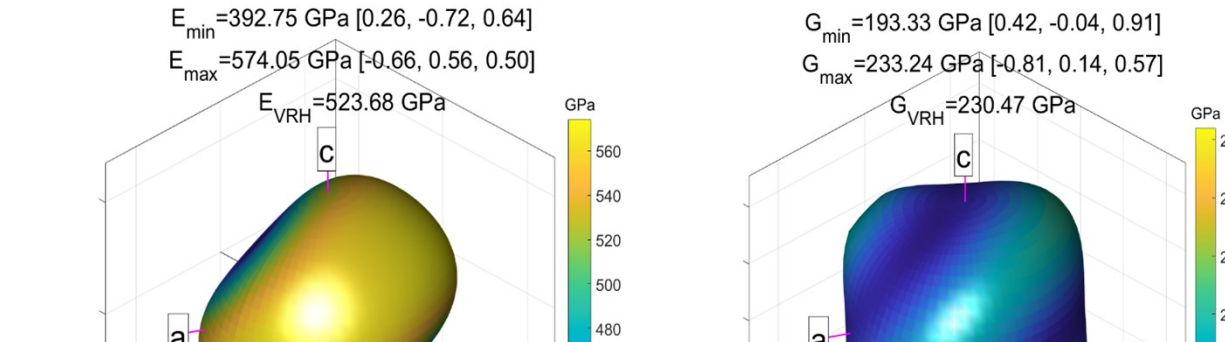

Linear compressibility (GPa^{-1})
min=1.15e-03, max=1.83e-03,
VRH$_{average}$ = 4.15e-03
c
a
b
GPa^{-1} ×10^{-3}
1.8
1.7
1.6
1.5
1.4
1.3
1.2

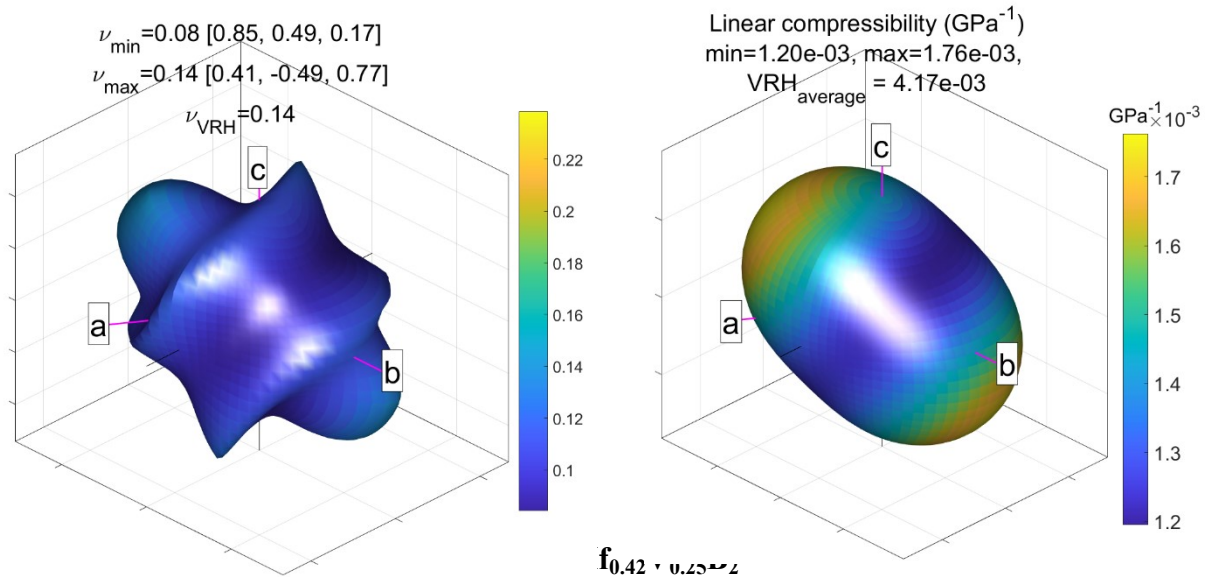

E_{min}=405.62 GPa [-0.62, 0.74, 0.26]
E_{max}=586.17 GPa [0.37, -0.53, 0.77]
E_{VRH}=534.58 GPa
c
GPa
580
560
540
520
500


G_{min}=192.99 GPa [-0.09, 1.00, 0.00]
G_{max}=247.70 GPa [0.75, 0.43, 0.50]
G_{VRH}=235.30 GPa
c
GPa
270
260
250
240
230

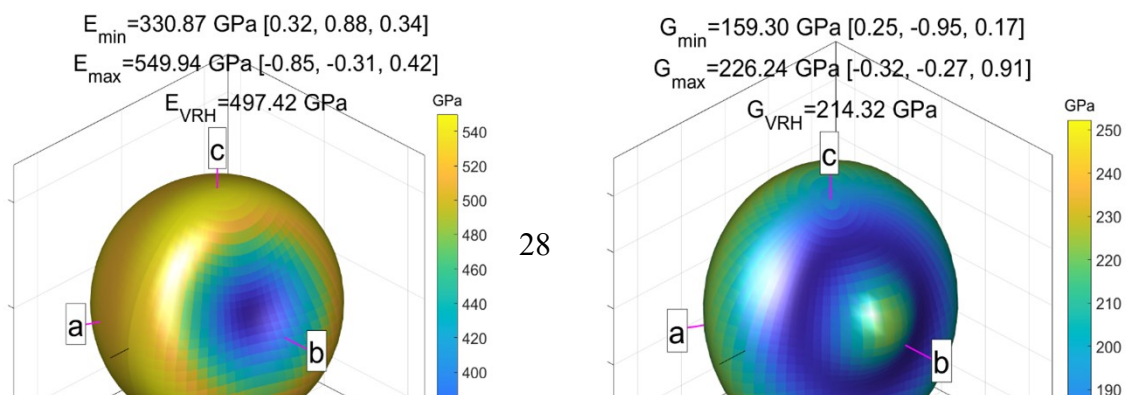


HEB-7 $Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B_2$

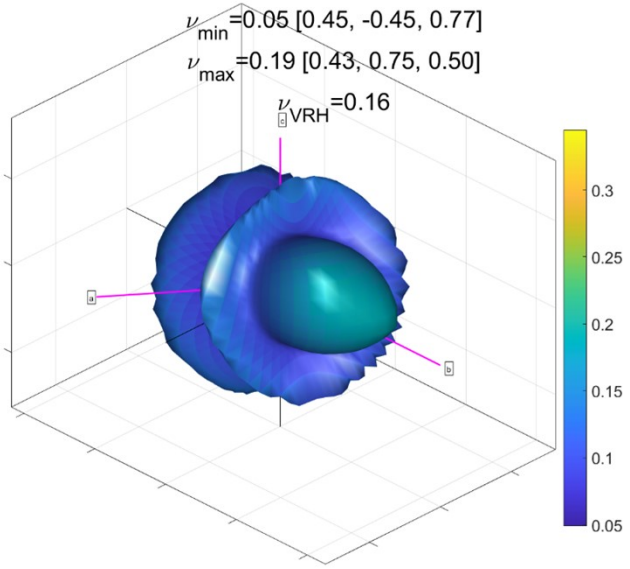


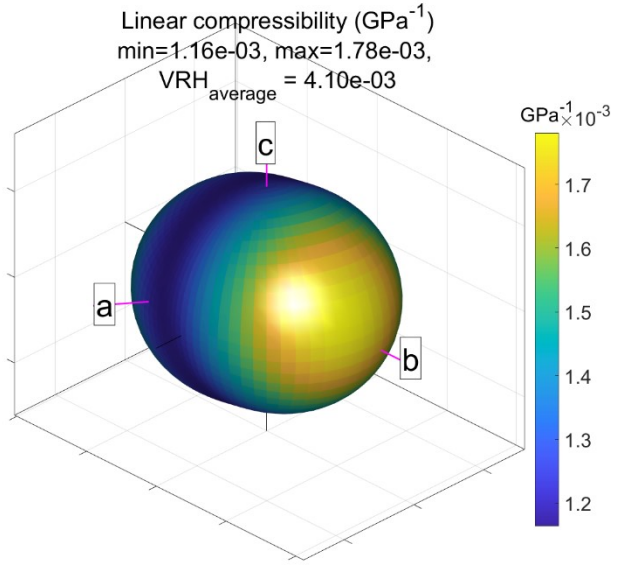


ν_{min}=0.08 [0.85, 0.49, 0.17]
ν_{max}=0.14 [0.41, -0.49, 0.77]
ν_{VRH}=0.14
Linear compressibility (GPa^{-1})
min=1.20e-03, max=1.76e-03,
$VRH_{average}$ = 4.17e-03
GPa^{-1} $\times 10^{-3}$

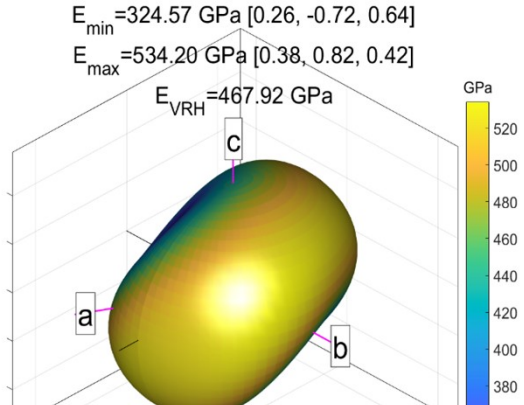


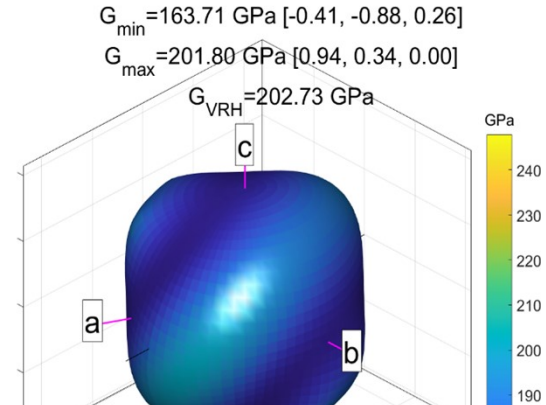
E_{min}=330.87 GPa [0.32, 0.88, 0.34]
E_{max}=549.94 GPa [-0.85, -0.31, 0.42]
E_{VRH}=497.42 GPa
G_{min}=159.30 GPa [0.25, -0.95, 0.17]
G_{max}=226.24 GPa [-0.32, -0.27, 0.91]
G_{VRH}=214.32 GPa
GPa

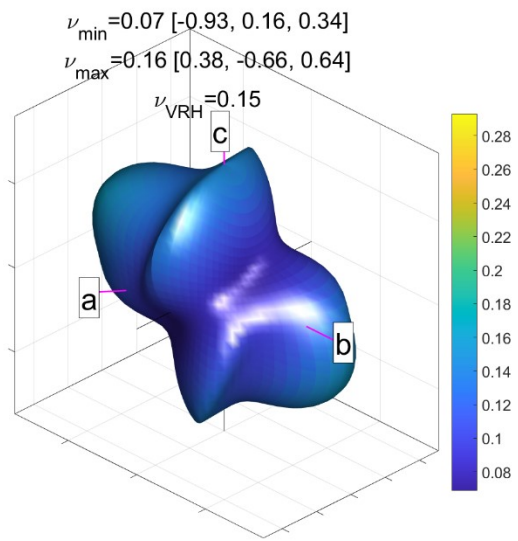


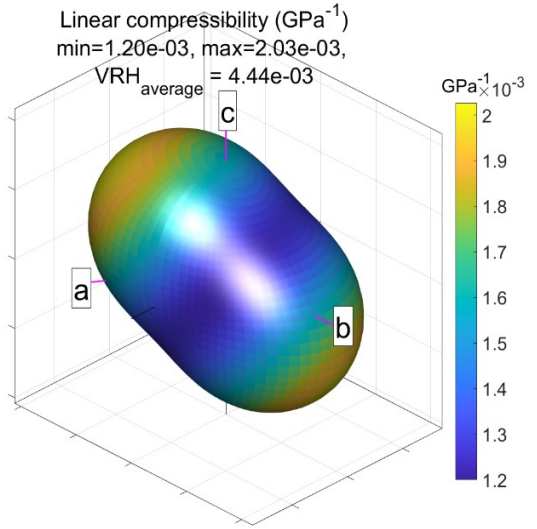


HEB-9 $Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B_2$

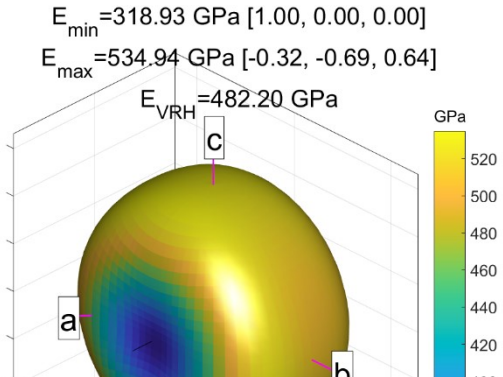


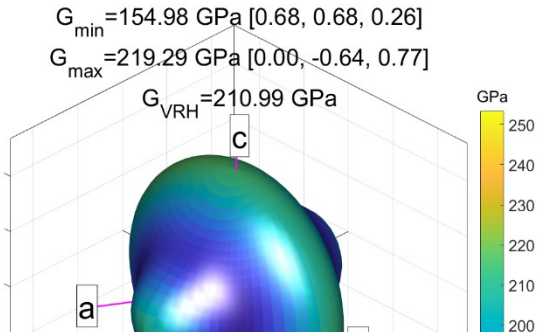


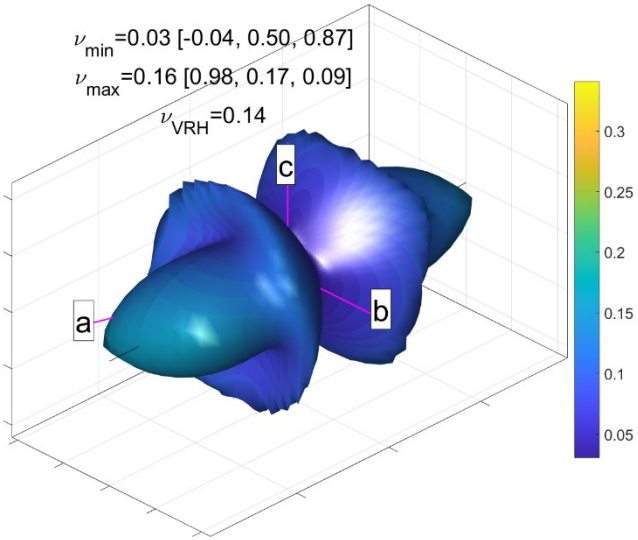


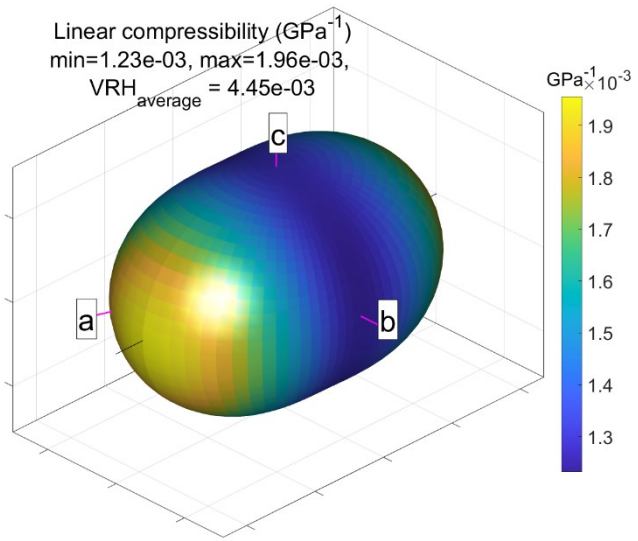


HEB-10 $Ti_{0.08}Zr_{0.33}Hf_{0.33}V_{0.25}B_2$

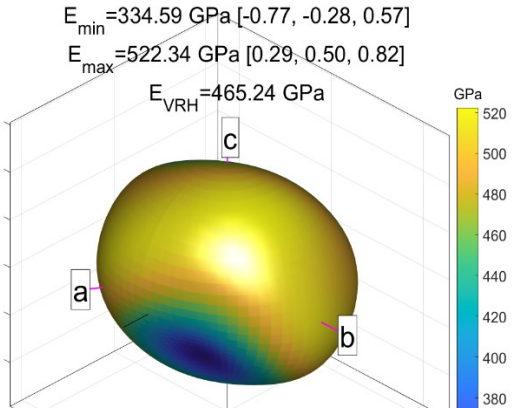


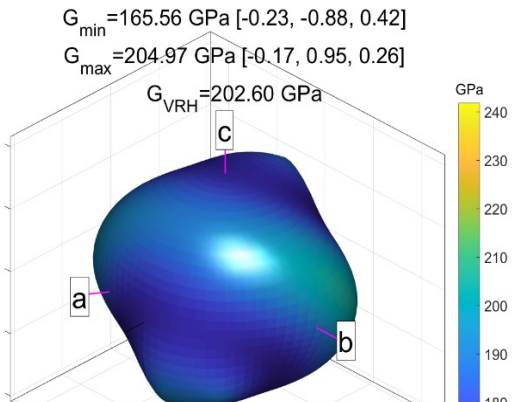


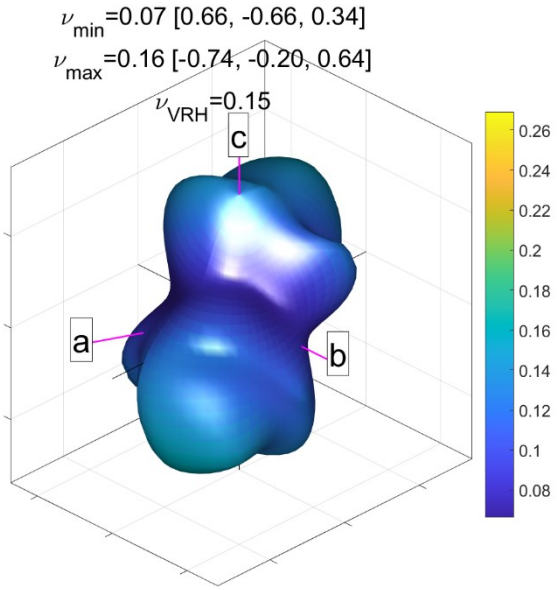


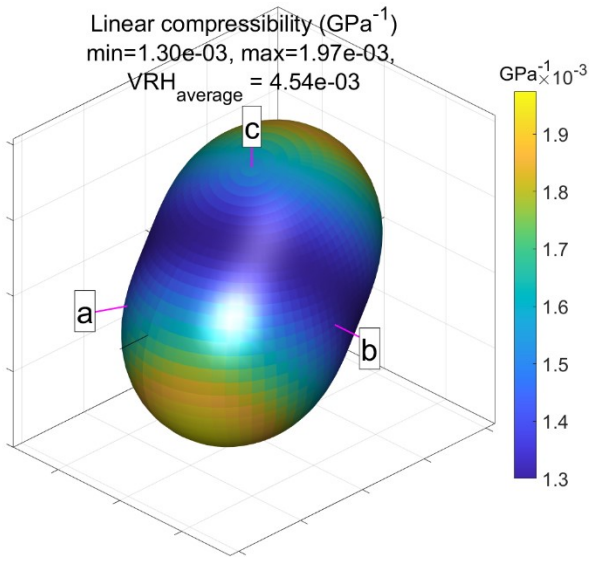


HEB-11 $Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B_2$

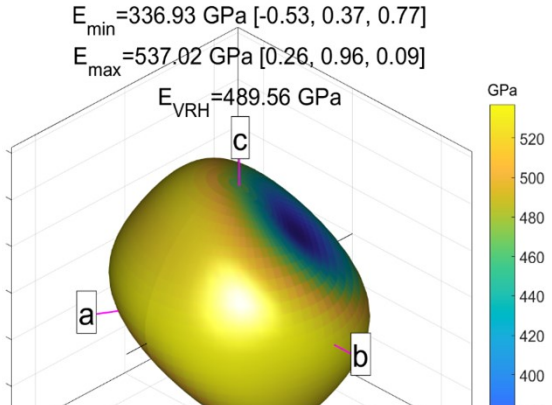


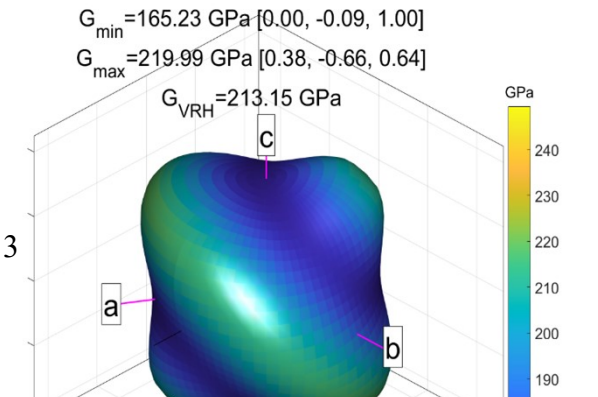


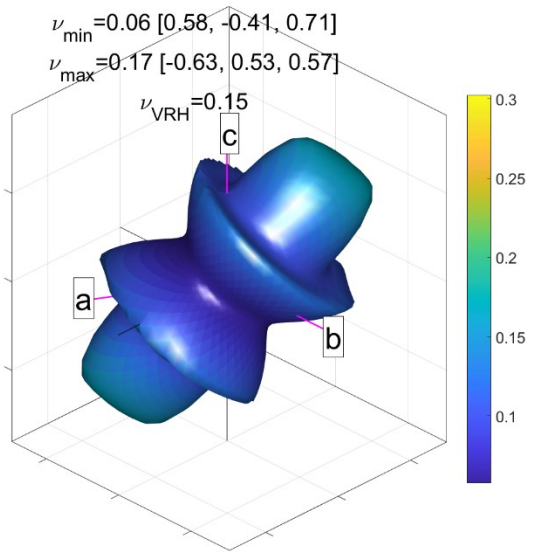


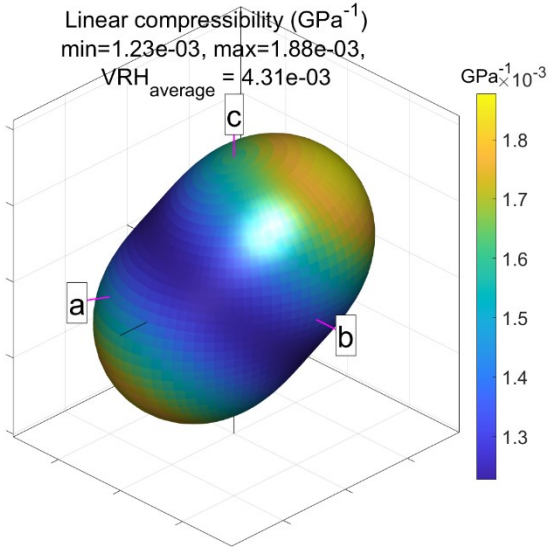


HEB-12 $Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B_2$

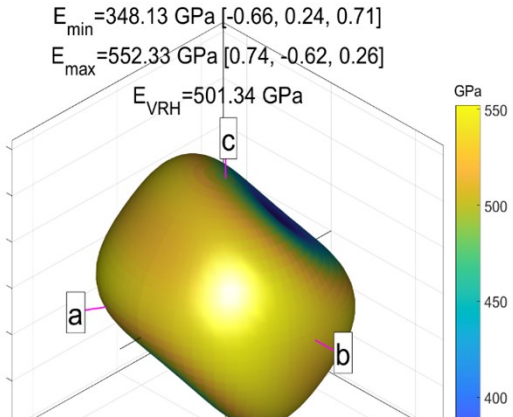


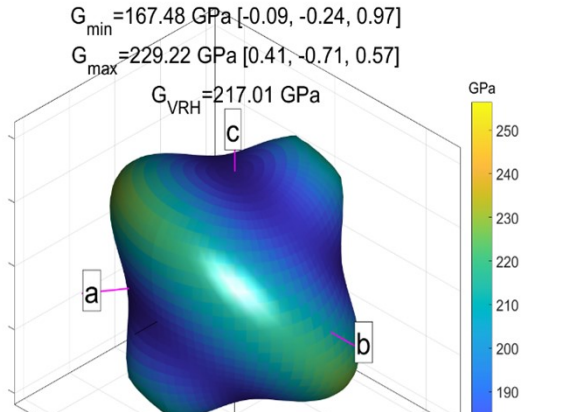


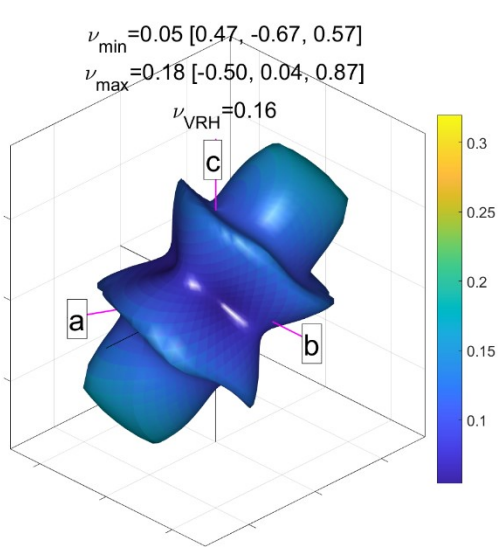


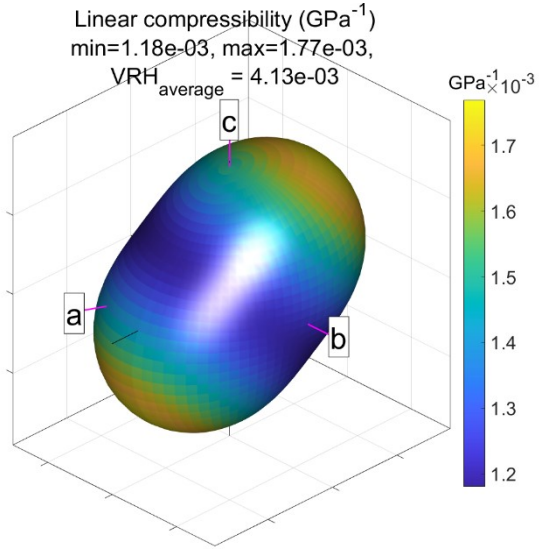


HEB-13 $Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B_2$

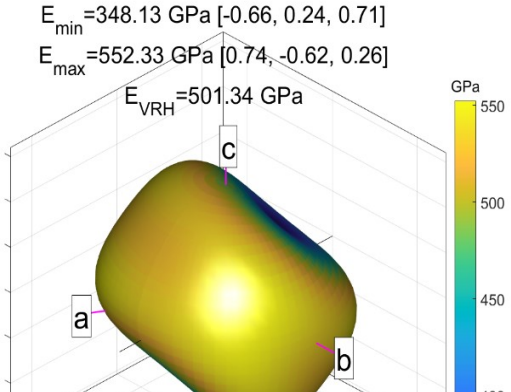


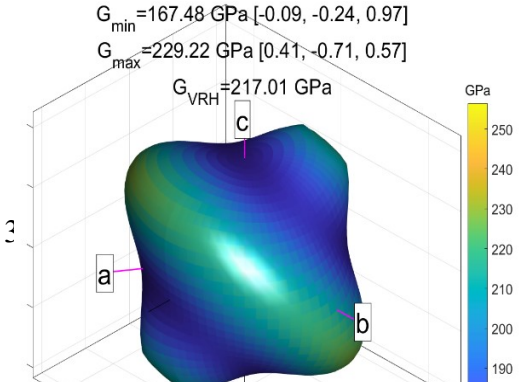


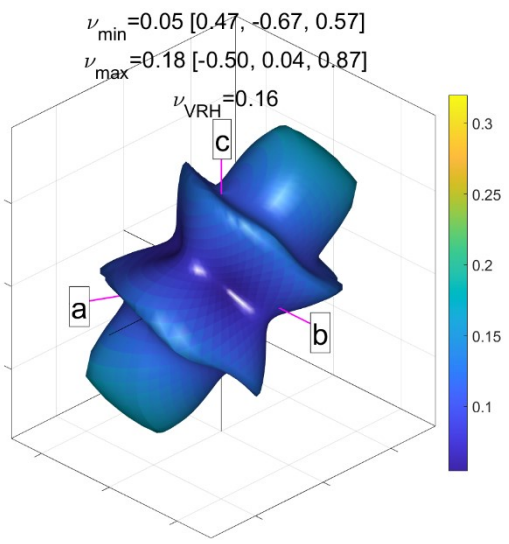


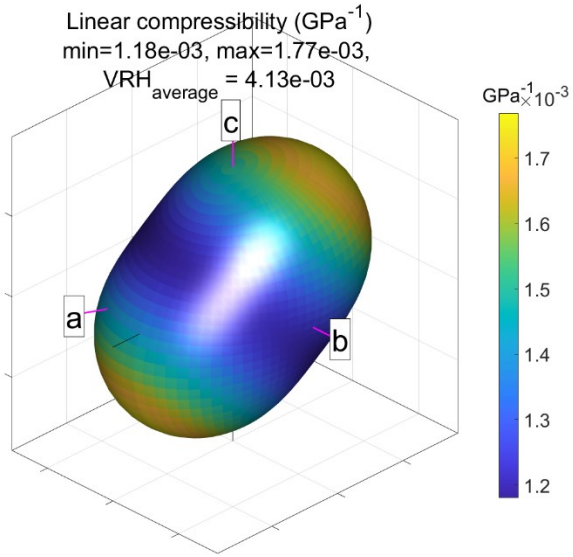


HEB-14 $Ti_{0.17}Zr_{0.25}Hf_{0.25}V_{0.33}B_2$

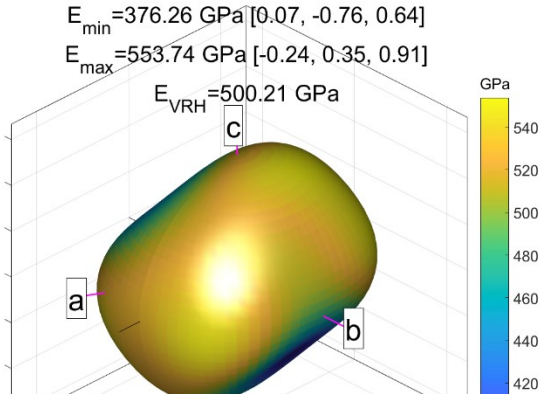


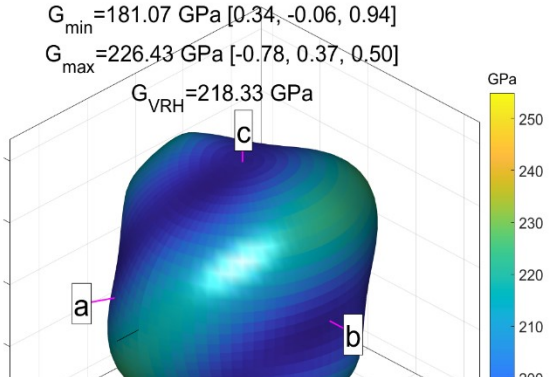


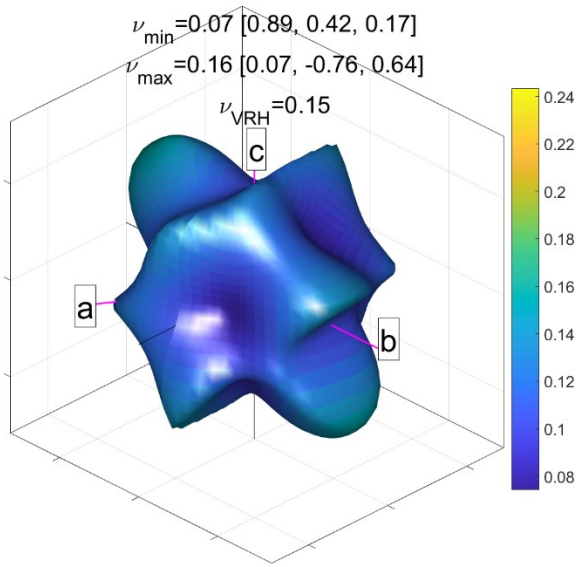


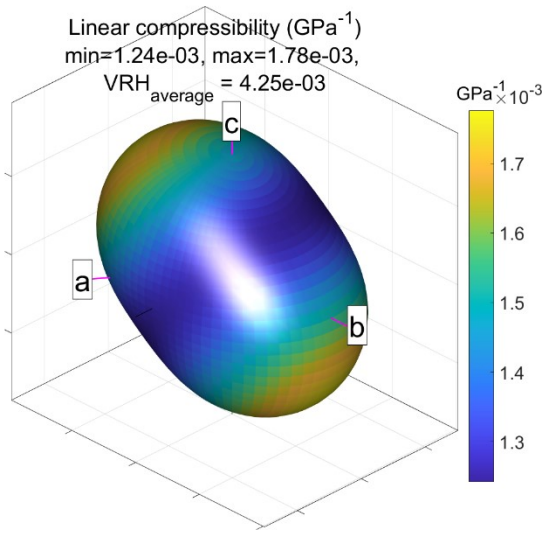


HEB-15 $Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B_2$

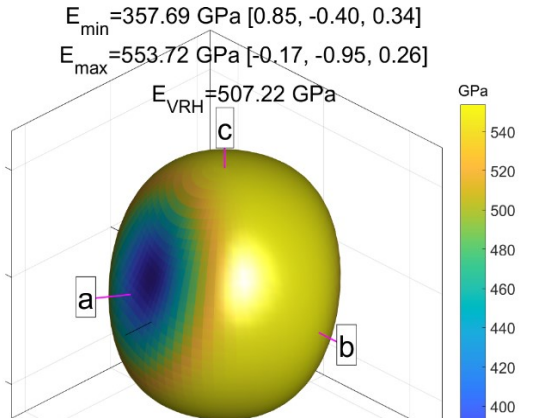


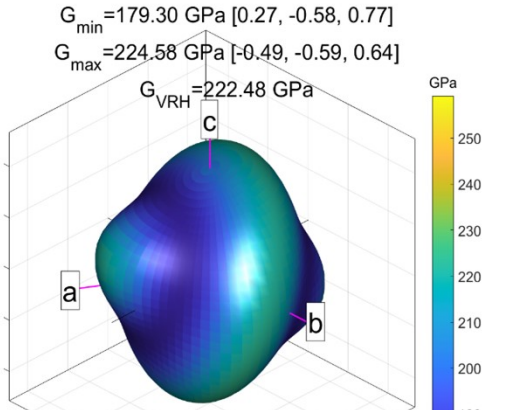


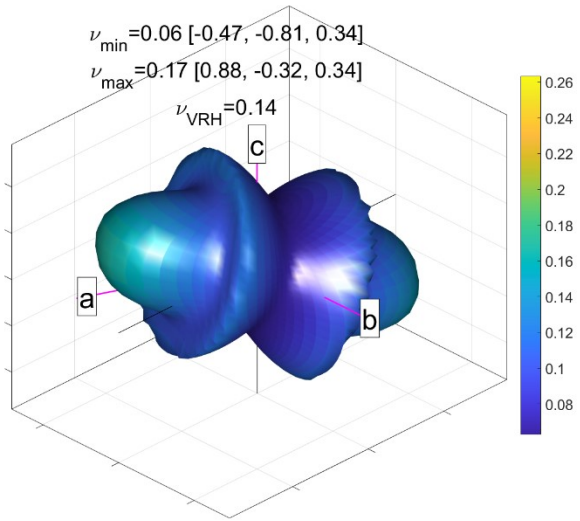

ν_{min}=0.07 [0.89, 0.42, 0.17]
ν_{max}=0.16 [0.07, -0.76, 0.64]
ν_{VRH}=0.15
c
a
b
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08

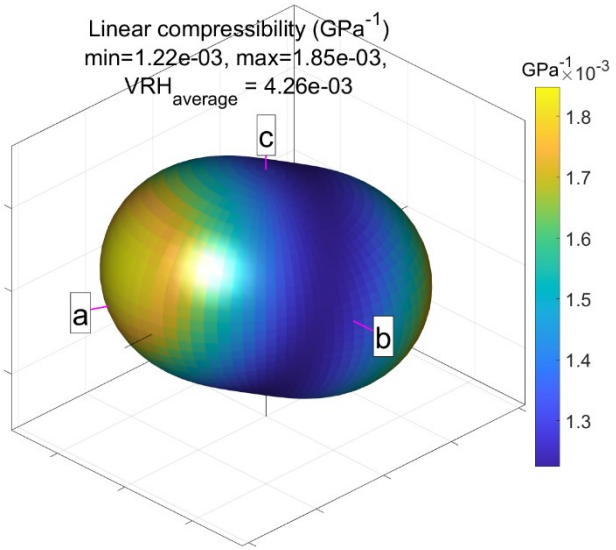

Linear compressibility (GPa^{-1})
min=1.24e-03, max=1.78e-03,
$VRH_{average}$ = 4.25e-03
c
a
b
GPa^{-1} ×10^{-3}
1.7
1.6
1.5
1.4
1.3

;Zr

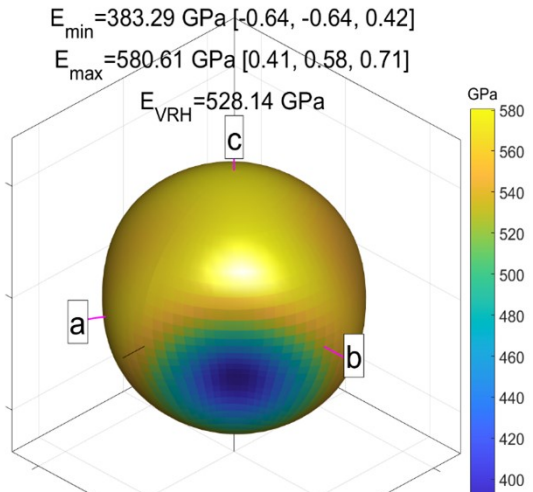

E_{min}=357.69 GPa [0.85, -0.40, 0.34]
E_{max}=553.72 GPa [-0.17, -0.95, 0.26]
E_{VRH}=507.22 GPa
c
a
b
GPa
540
520
500
480
460
440
420
400

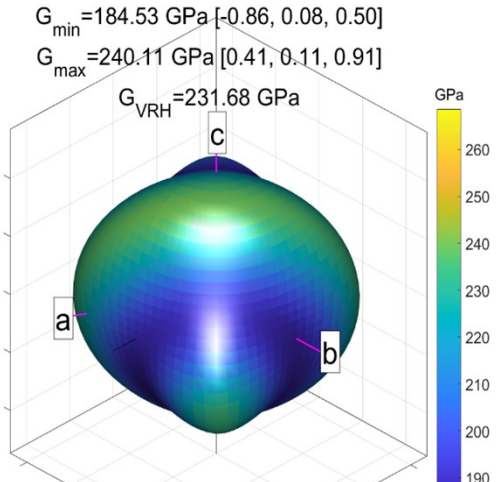

G_{min}=179.30 GPa [0.27, -0.58, 0.77]
G_{max}=224.58 GPa [-0.49, -0.59, 0.64]
G_{VRH}=222.48 GPa
c
a
b
GPa
250
240
230
220
210
200

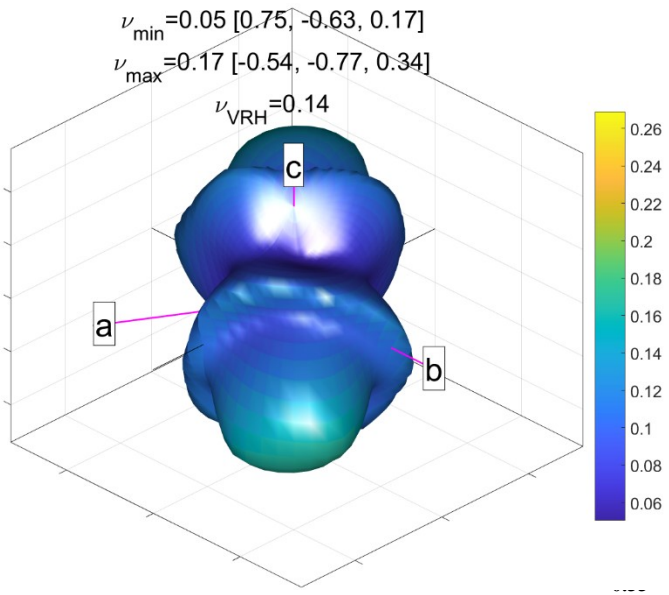


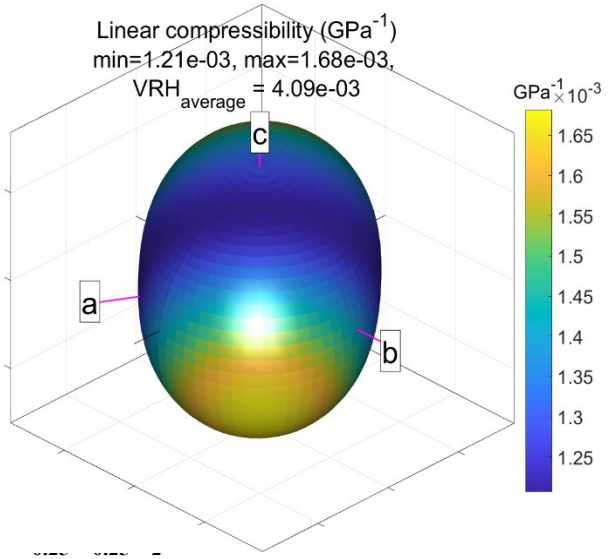


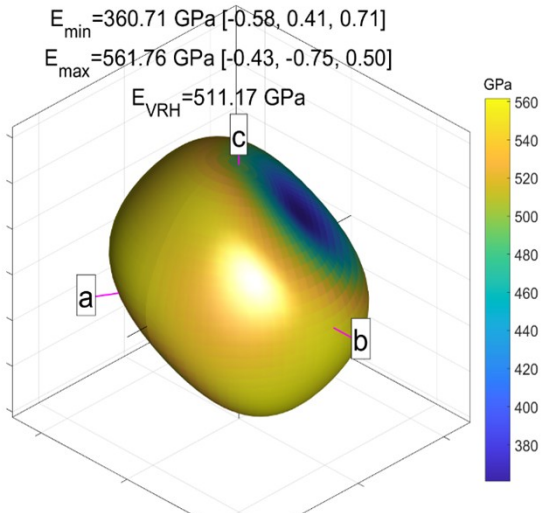
HEB-17 $Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B_2$

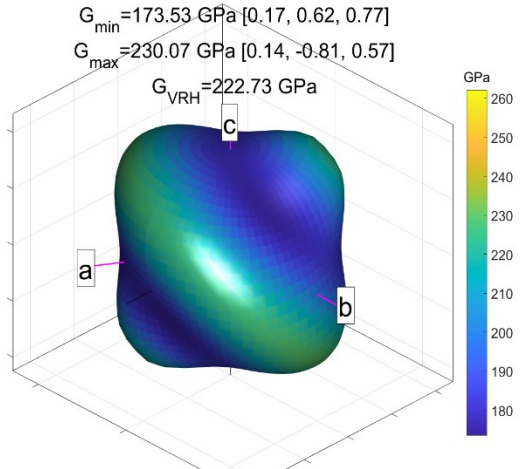


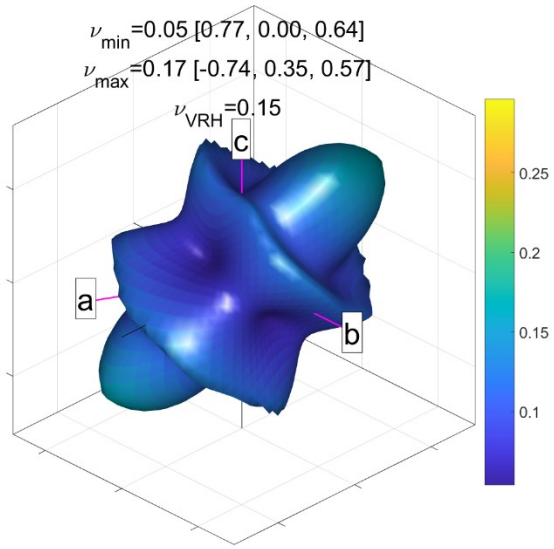


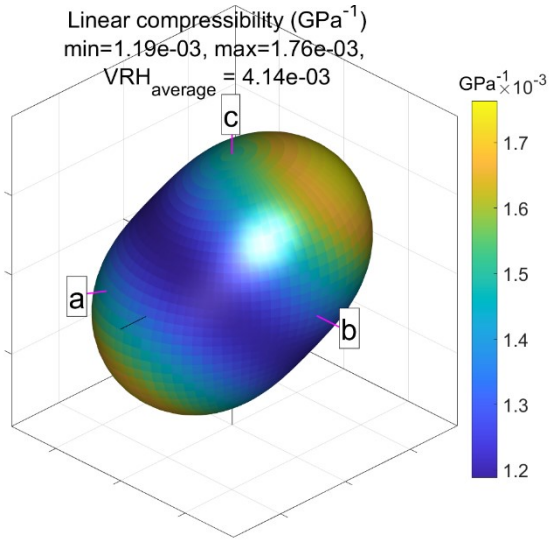

ν_{min}=0.05 [0.75, -0.63, 0.17]
ν_{max}=0.17 [-0.54, -0.77, 0.34]
ν_{VRH}=0.14
c
a
b
0.26
0.24
0.22
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06


Linear compressibility (GPa^{-1})
min=1.21e-03, max=1.68e-03,
VRH$_{average}$ = 4.09e-03
c
a
b
GPa^{-1} ×10^{-3}
1.65
1.6
1.55
1.5
1.45
1.4
1.35
1.3
1.25

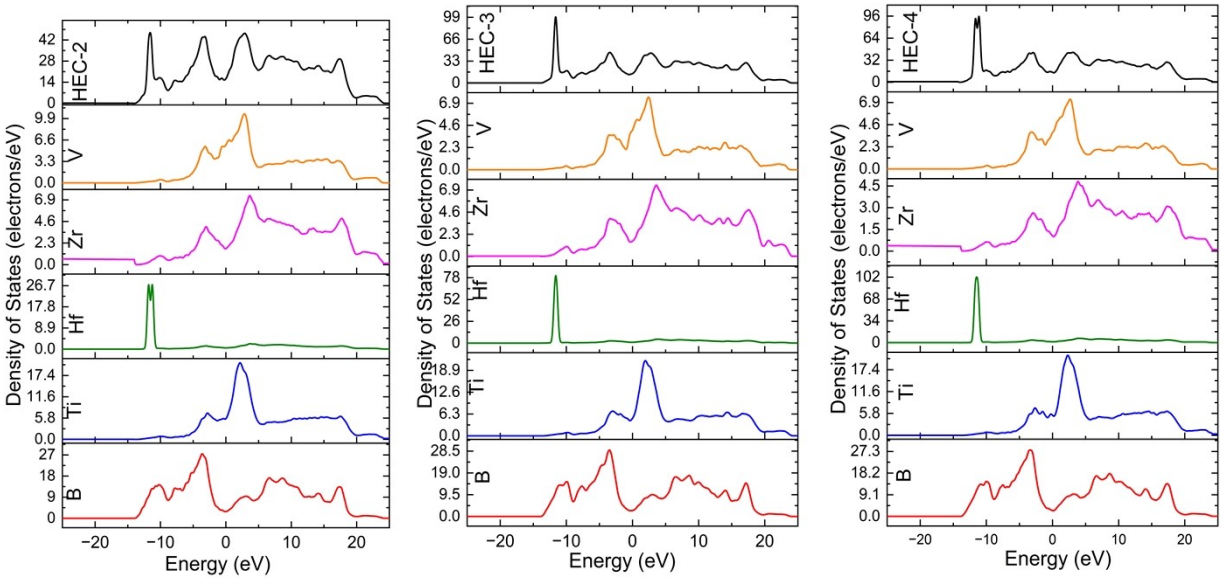

E_{min}=360.71 GPa [-0.58, 0.41, 0.71]
E_{max}=561.76 GPa [-0.43, -0.75, 0.50]
E_{VRH}=511.17 GPa
c
a
b
GPa
560
540
520
500
480
460
440
420
400
380

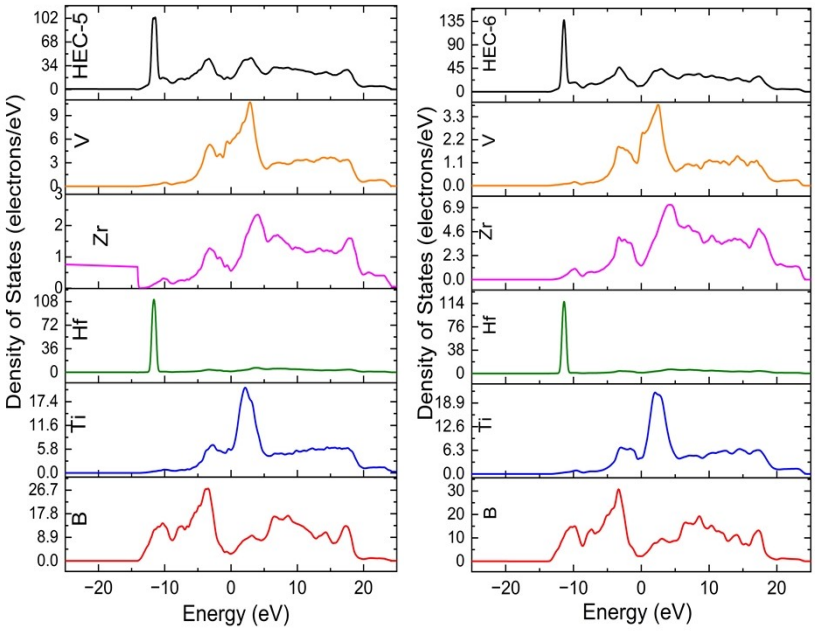

G_{min}=173.53 GPa [0.17, 0.62, 0.77]
G_{max}=230.07 GPa [0.14, -0.81, 0.57]
G_{VRH}=222.73 GPa
c
a
b
GPa
260
250
240
230
220
210
200
190
180


ν_{min}=0.05 [0.77, 0.00, 0.64]
ν_{max}=0.17 [-0.74, 0.35, 0.57]
ν_{VRH}=0.15
c
a
b
0.25
0.2
0.15
0.1

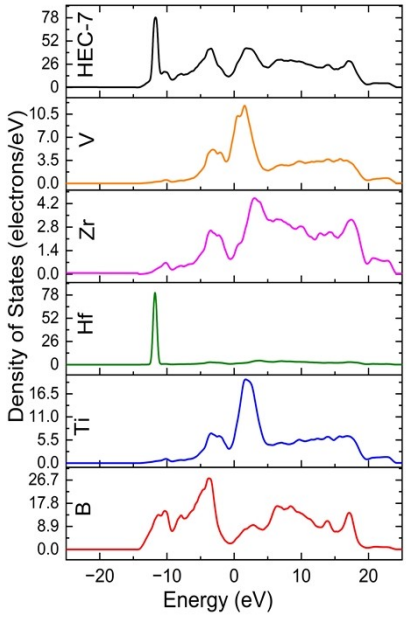

Linear compressibility (GPa^{-1})
min=1.19e-03, max=1.76e-03,
VRH$_{average}$ = 4.14e-03
GPa^{-1} ×10^{-3}
c
a
b
1.7
1.6
1.5
1.4
1.3
1.2

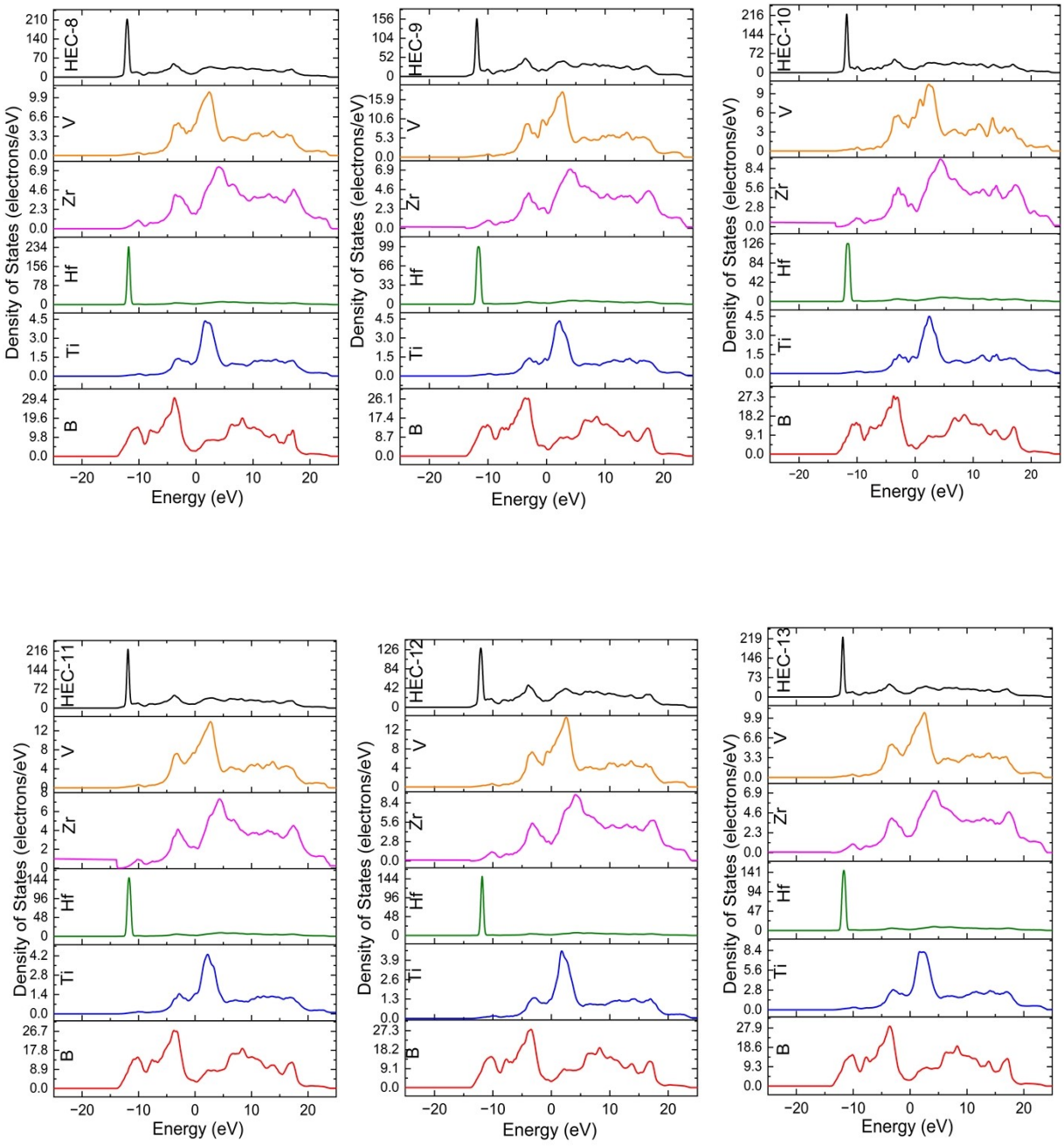
S 3. Total density of states and Projected density of states of HEBs

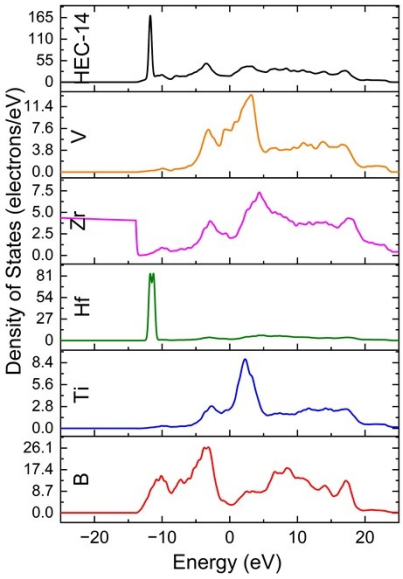


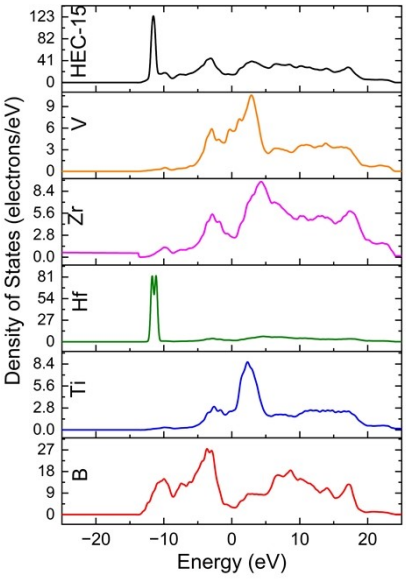

HEC-5
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

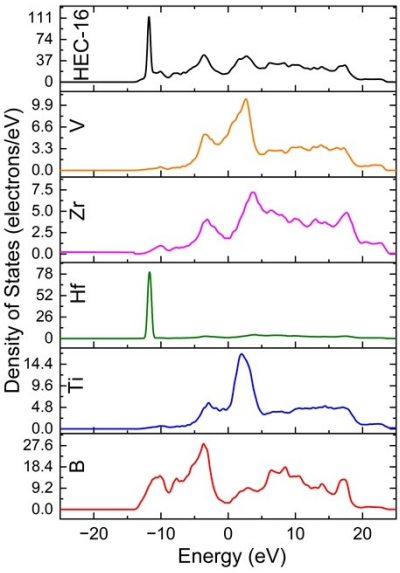
HEC-6
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

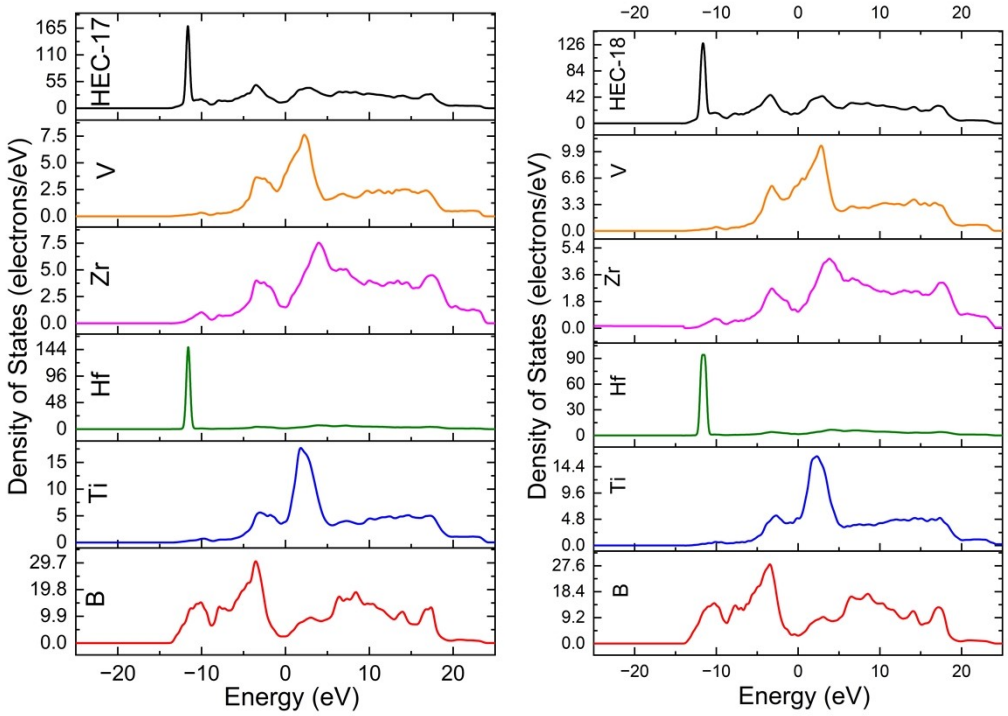

HEC-7
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)


HEC-8
HEC-9
HEC-10
HEC-11
HEC-12
HEC-13
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

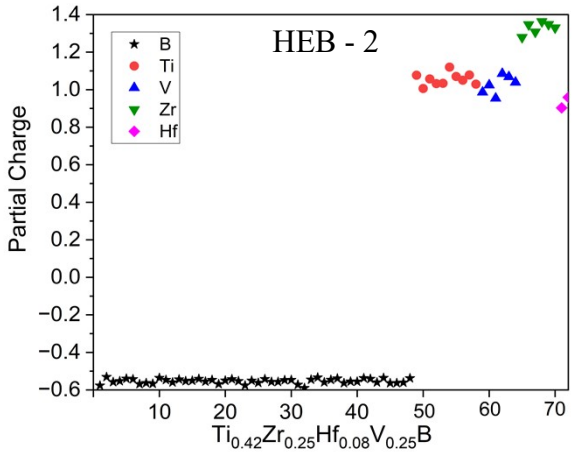

HEC-14
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

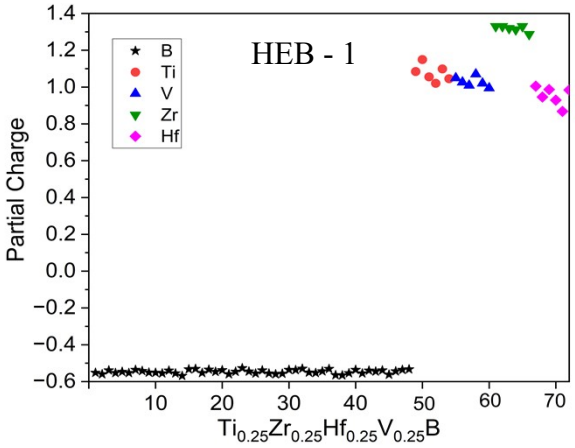

HEC-15
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

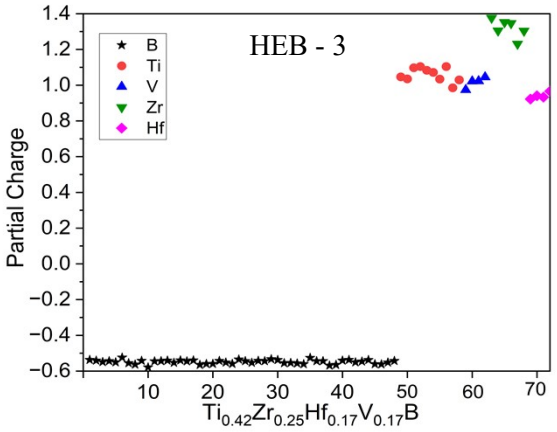

HEC-16
V
Zr
Hf
Ti
B
Density of States (electrons/eV)
Energy (eV)

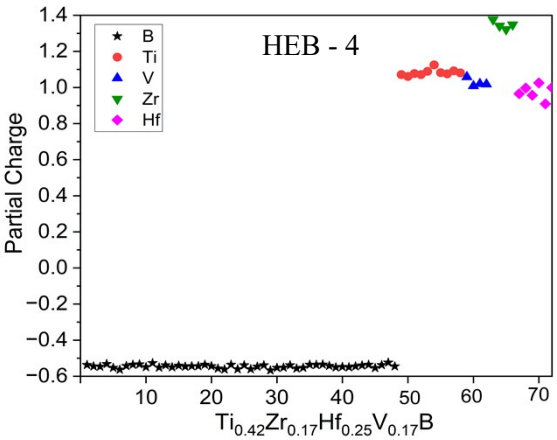


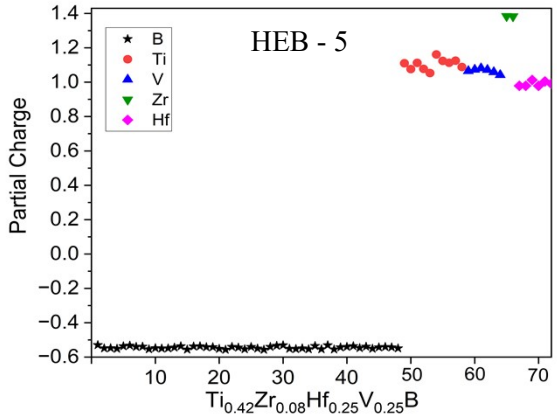
S 4. Mulliken partial charge analysis of HEBs

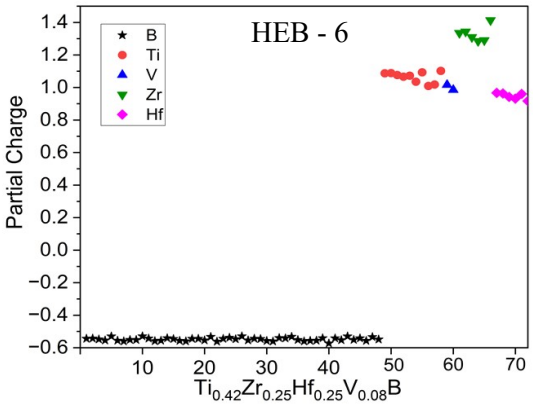



HEB - 1
B
Ti
V
Zr
Hf
Partial Charge
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
10
20
30
40
50
60
70
Ti0.25Zr0.25Hf0.25V0.25B

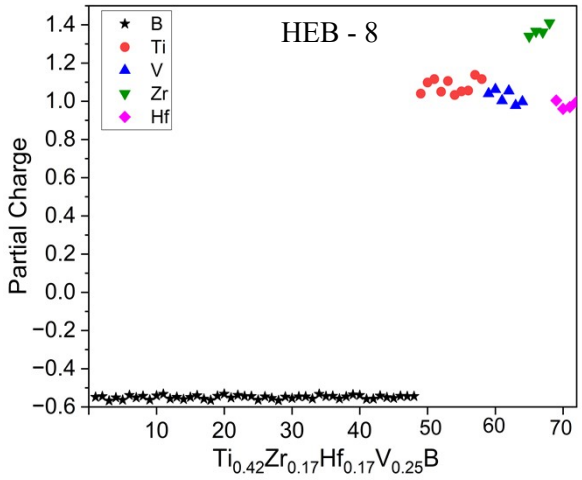

HEB - 3
B
Ti
V
Zr
Hf
Partial Charge
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
10
20
30
40
50
60
70
Ti0.42Zr0.25Hf0.17V0.17B

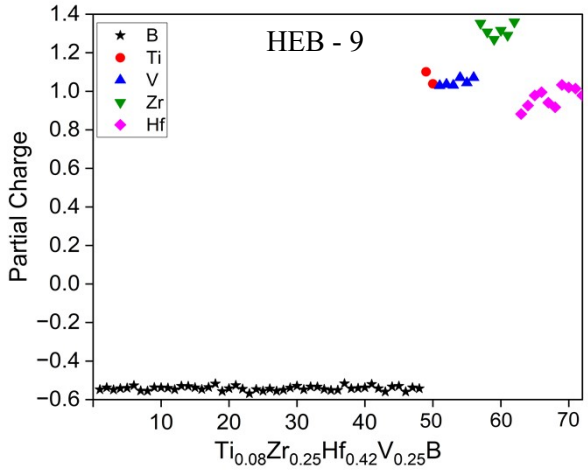

HEB - 4
B
Ti
V
Zr
Hf
Partial Charge
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
10
20
30
40
50
60
70
Ti0.42Zr0.17Hf0.25V0.17B

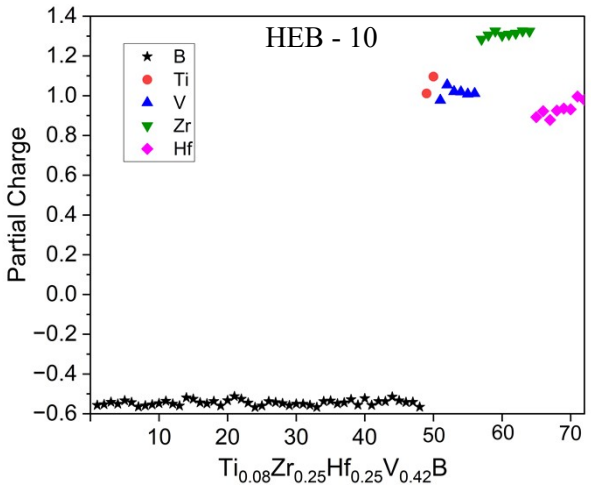

HEB - 5
B
Ti
V
Zr
Hf
Partial Charge
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
10
20
30
40
50
60
70
Ti0.42Zr0.08Hf0.25V0.25B

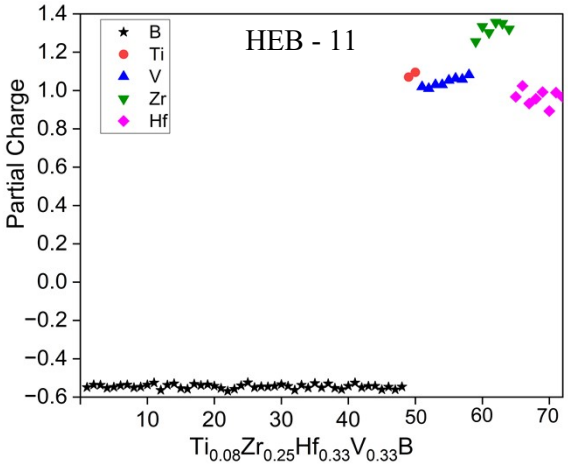

HEB - 6
B
Ti
V
Zr
Hf
Partial Charge
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.6
10
20
30
40
50
60
70
Ti0.42Zr0.25Hf0.25V0.08B

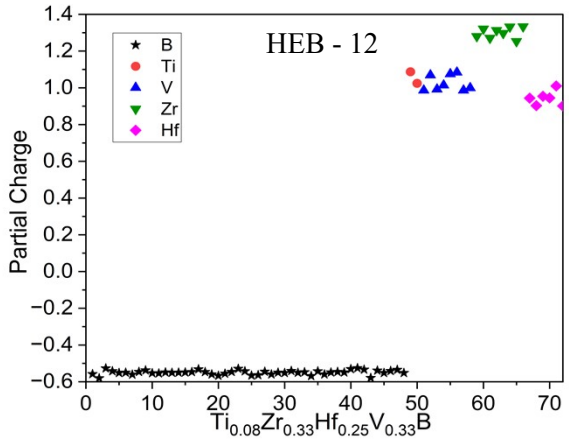
HEB - 7


HEB - 8
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B$

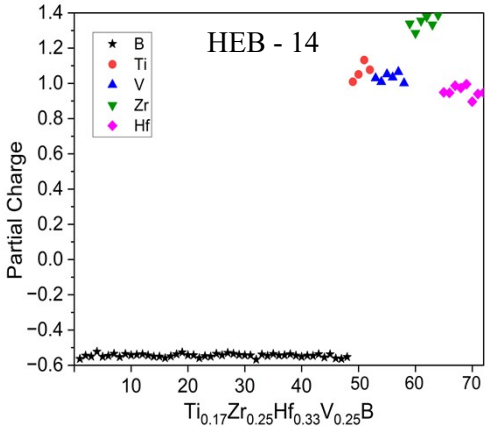

HEB - 9
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.08}Zr_{0.25}Hf_{0.42}V_{0.25}B$

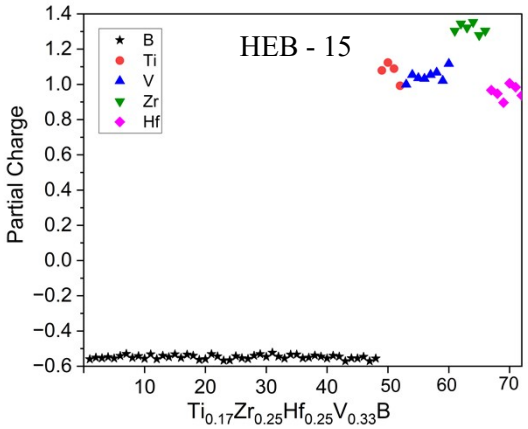

HEB - 10
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B$

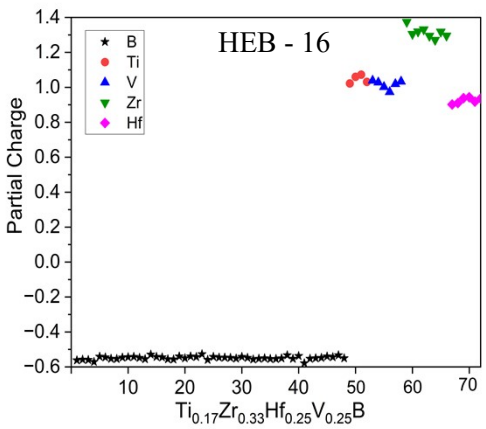

HEB - 11
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B$

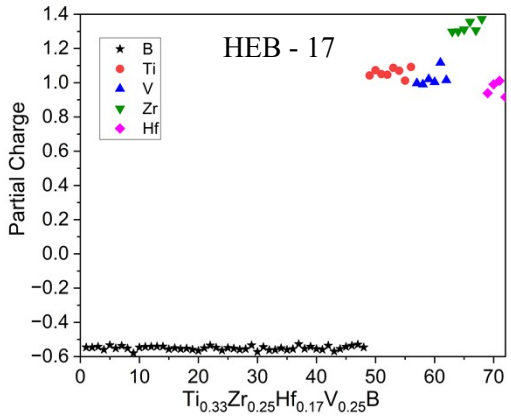

HEB - 12
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B$

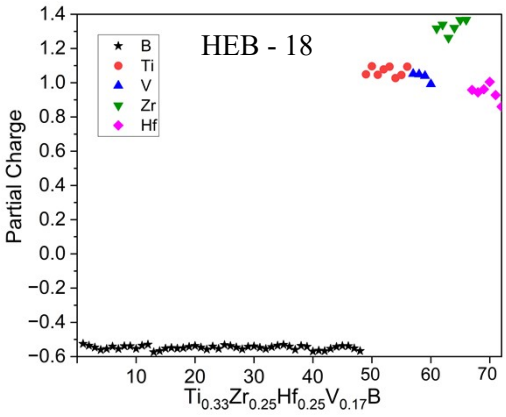
HEB - 13


HEB - 14
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B$

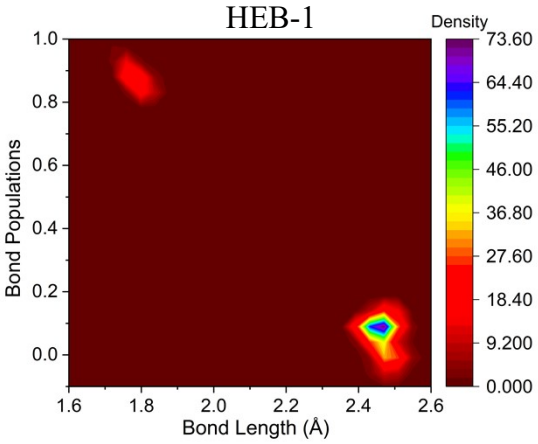

HEB - 15
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.17}Zr_{0.25}Hf_{0.25}V_{0.33}B$


HEB - 16
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B$

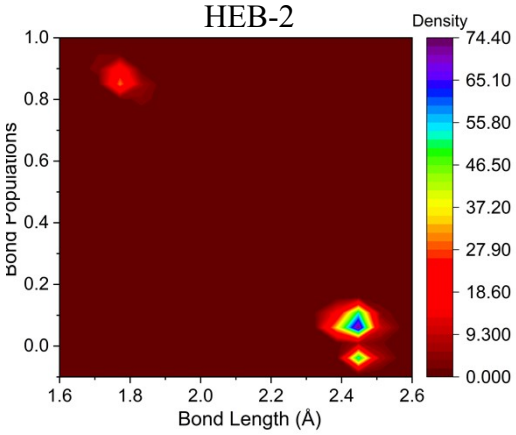

HEB - 17
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.33}Zr_{0.25}Hf_{0.17}V_{0.25}B$


HEB - 18
B
Ti
V
Zr
Hf
Partial Charge
$Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B$

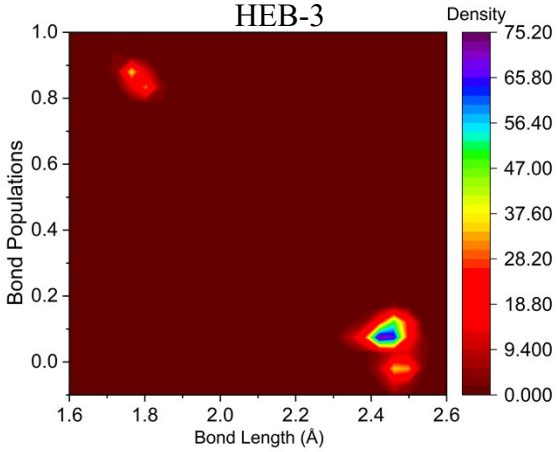
S 5. Bond population and bond length analysis of HEBs



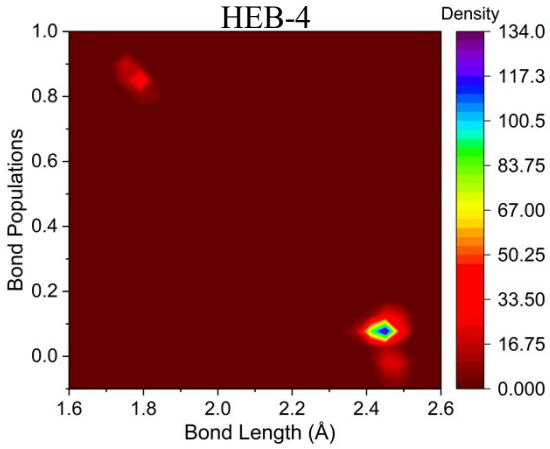
$Ti_{0.25}Zr_{0.25}Hf_{0.25}V_{0.25}B$



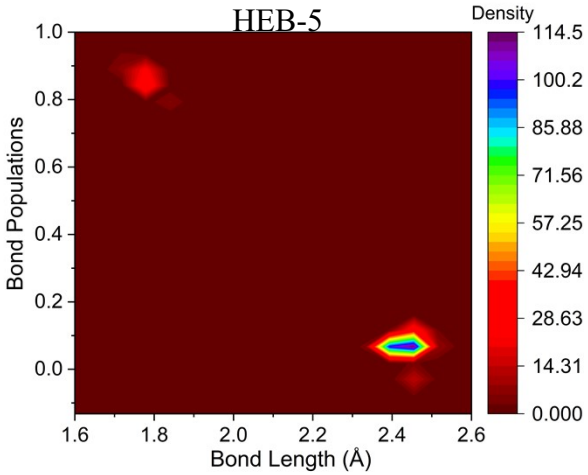
$Ti_{0.42}Zr_{0.25}Hf_{0.08}V_{0.25}B$



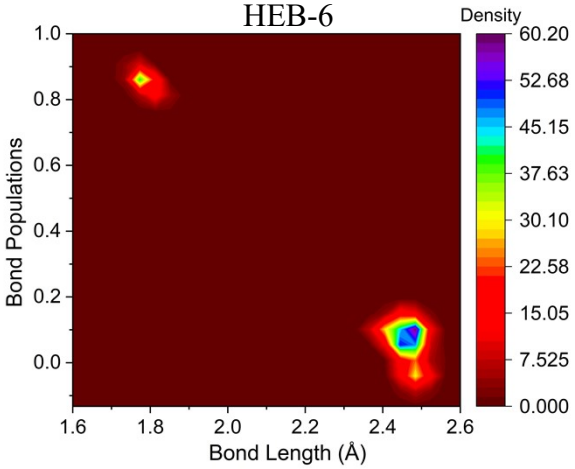
$Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B$



$Ti_{0.42}Zr_{0.17}Hf_{0.25}V_{0.17}B$



$Ti_{0.42}Zr_{0.08}Hf_{0.25}V_{0.25}B$



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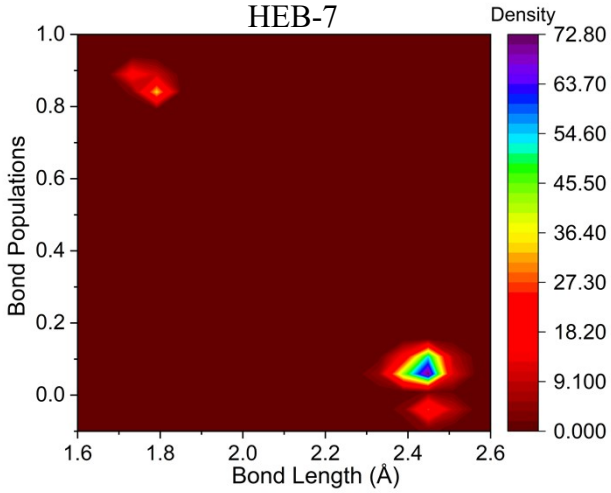
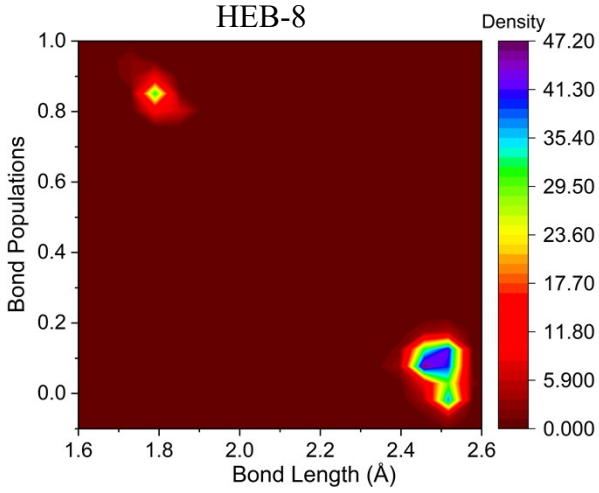
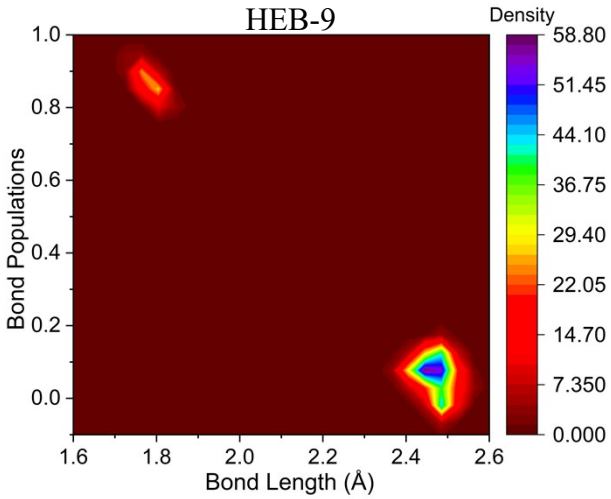


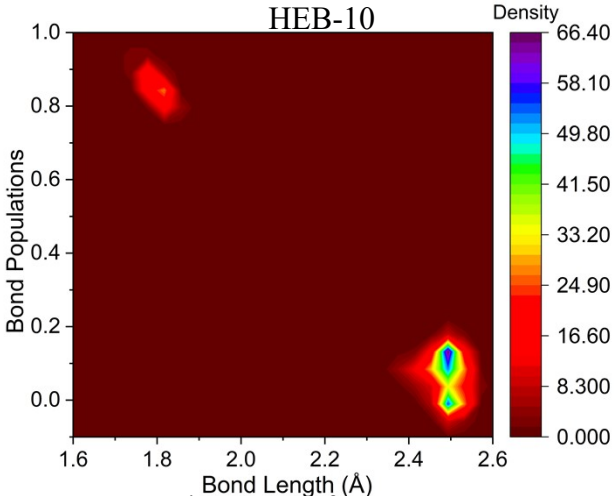
$Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B$



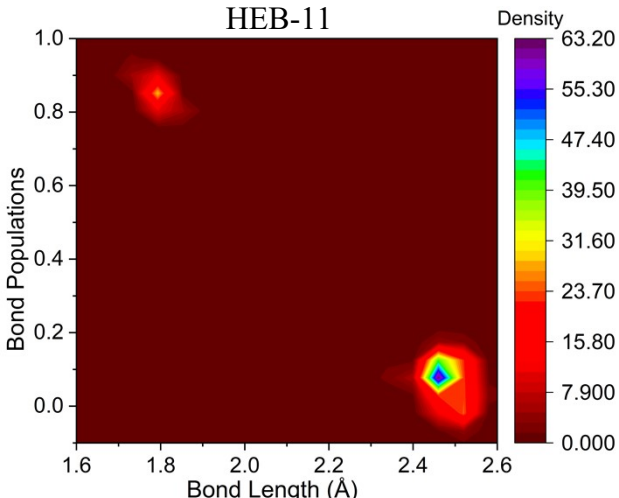
$Ti_{0.08}Zr_{0.25}Hf_{0.42}V_{0.25}B$



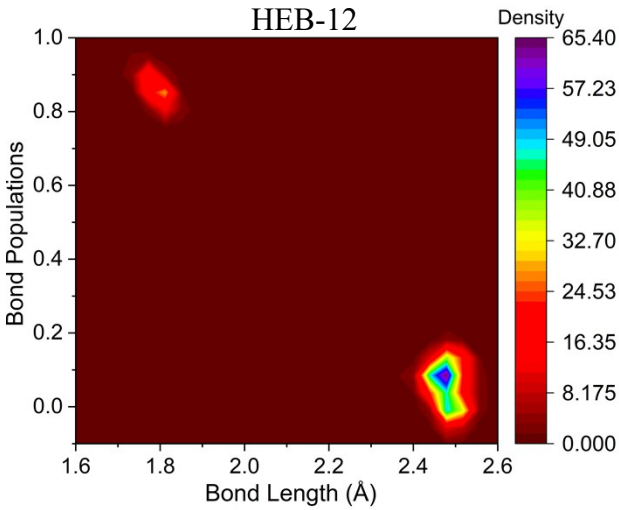
$Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B$



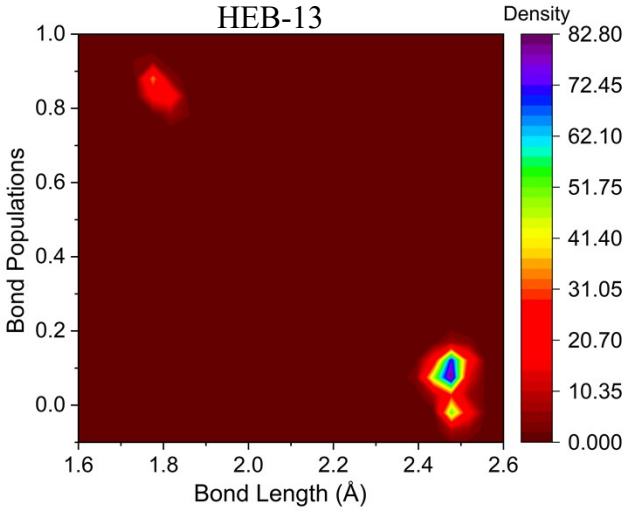
$Ti_{0.08}Zr_{0.33}Hf_{0.33}V_{0.25}B$



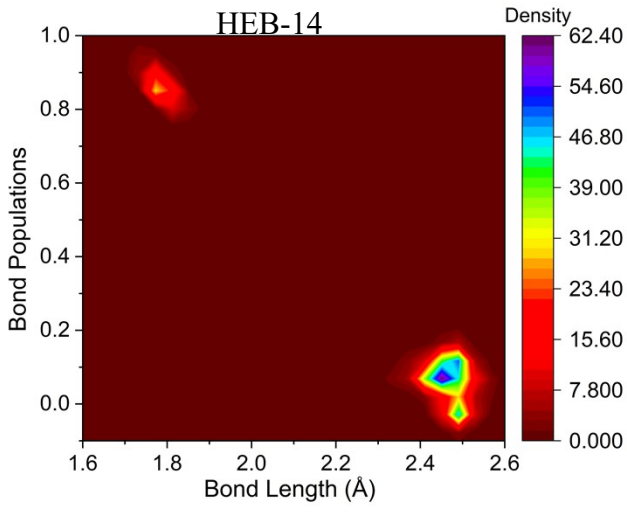
$Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B$



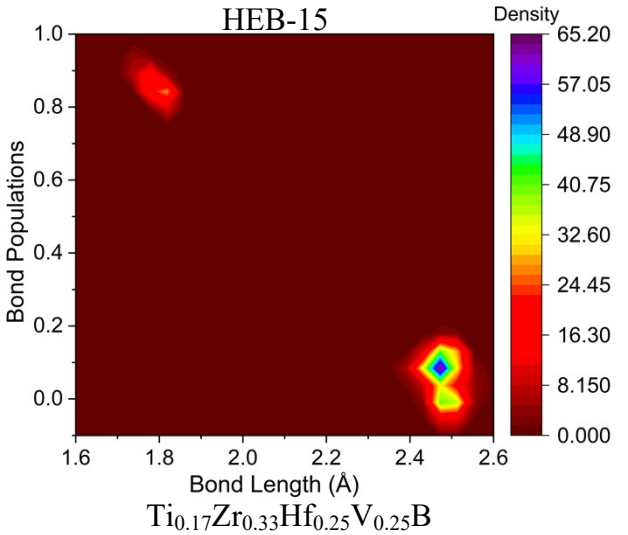
$Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B$



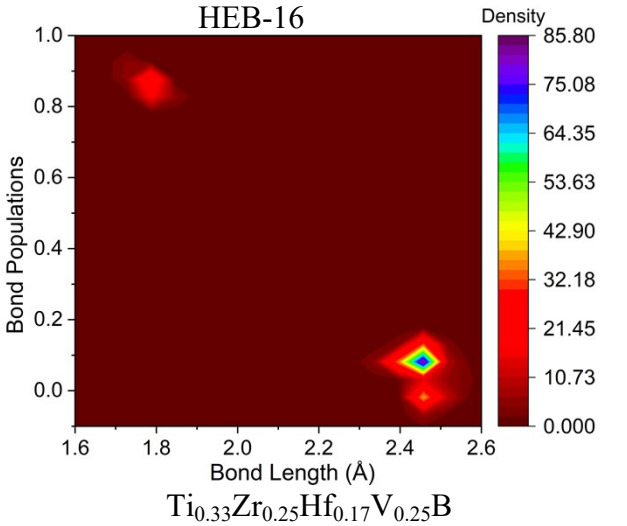
$Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B$



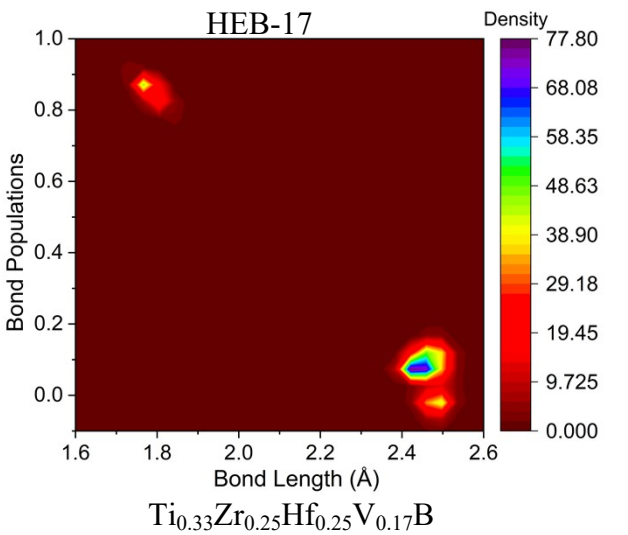
$Ti_{0.17}Zr_{0.25}Hf_{0.25}V_{0.33}B$



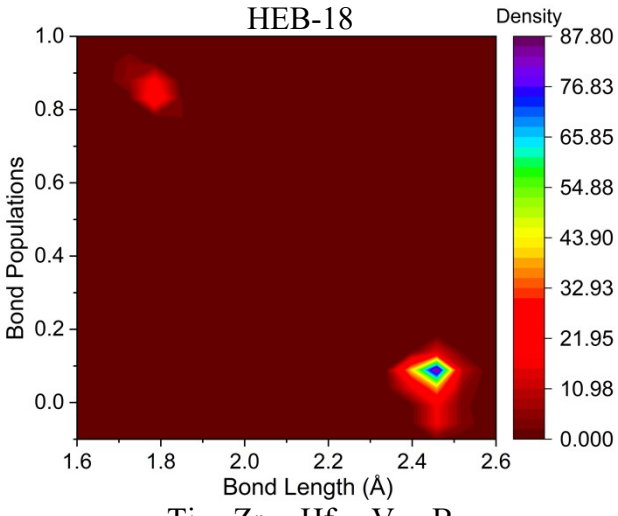
$Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B$



$Ti_{0.33}Zr_{0.25}Hf_{0.17}V_{0.25}B$

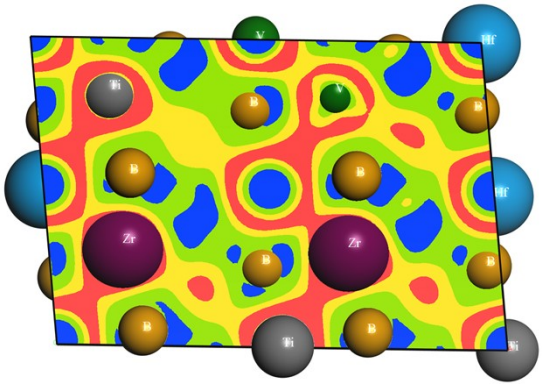


$Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B$

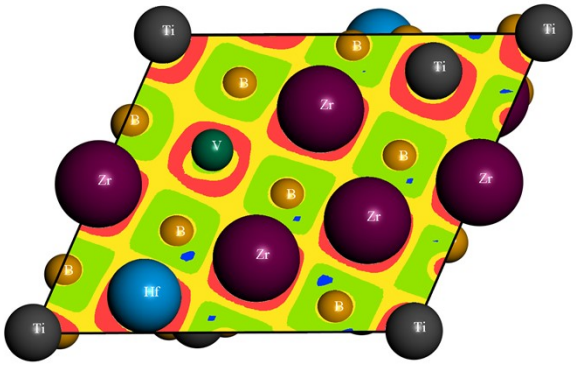


$Ti_{0.33}Zr_{0.17}Hf_{0.25}V_{0.25}B$

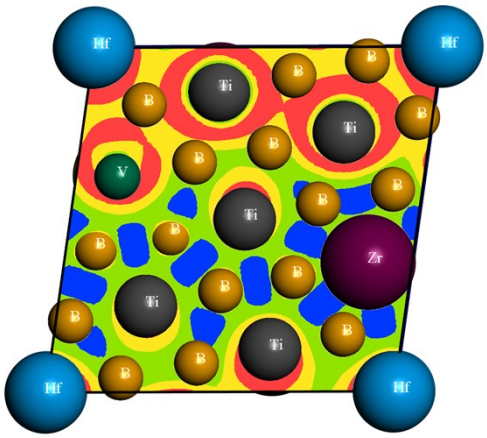
S 6. Electron localization function of HEBs



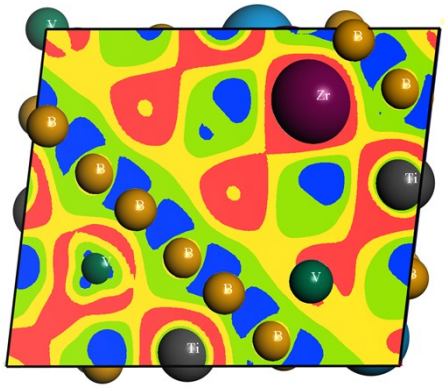
HEB - 1 ($Ti_{0.25}Zr_{0.25}Hf_{0.25}V_{0.25}B_2$)



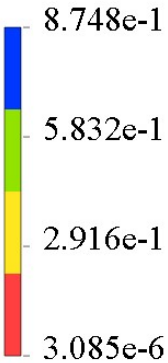
HEB - 2 ($Ti_{0.42}Zr_{0.25}Hf_{0.08}V_{0.25}B_2$)

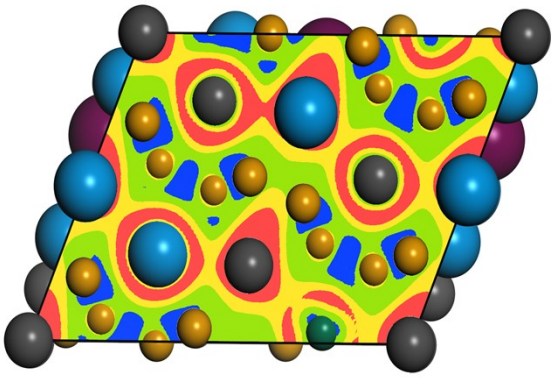


HEB – 3 ($Ti_{0.42}Zr_{0.25}Hf_{0.17}V_{0.17}B_2$)

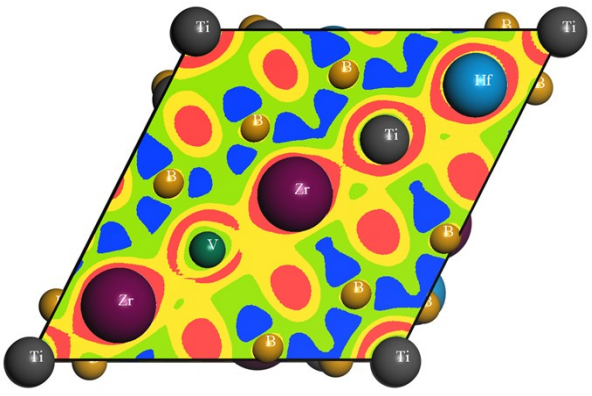


HEB – 4 ($Ti_{0.42}Zr_{0.17}Hf_{0.25}V_{0.17}B_2$)

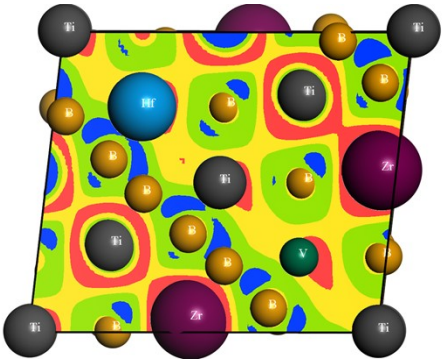




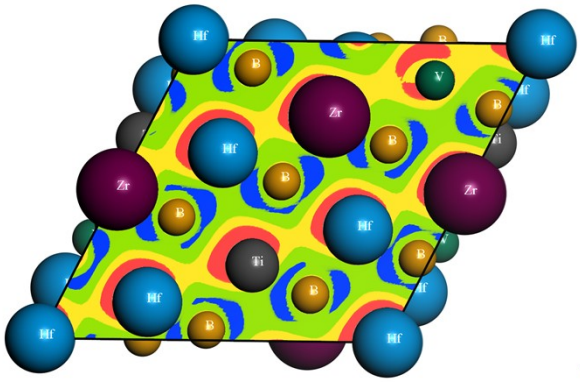
HEB – 5 ($Ti_{0.42}Zr_{0.08}Hf_{0.25}V_{0.25}B_2$)



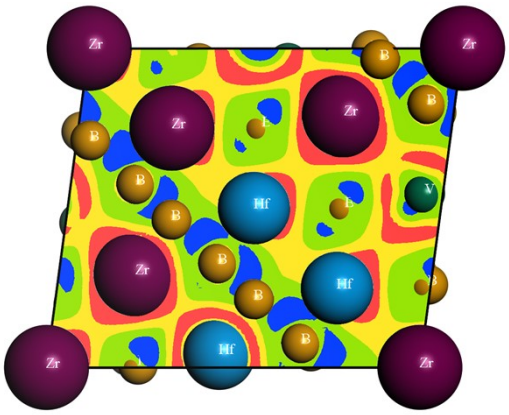
HEB – 6 ($Ti_{0.42}Zr_{0.25}Hf_{0.25}V_{0.08}B_2$)



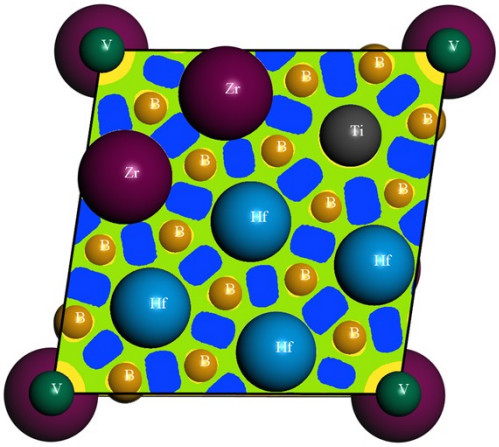
HEB – 7 ($Ti_{0.42}Zr_{0.17}Hf_{0.17}V_{0.25}B$)



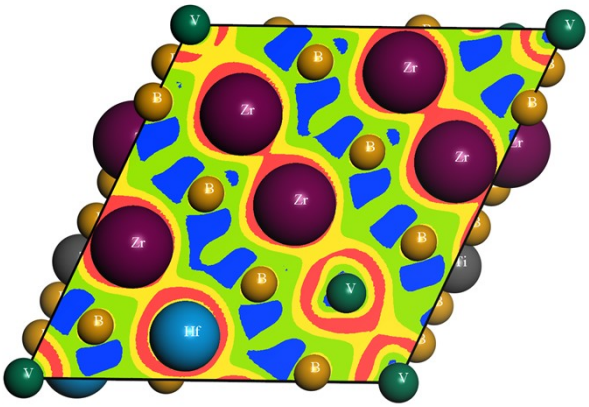
HEB – 8 ($Ti_{0.08}Zr_{0.25}Hf_{0.42}V_{0.25}B$)



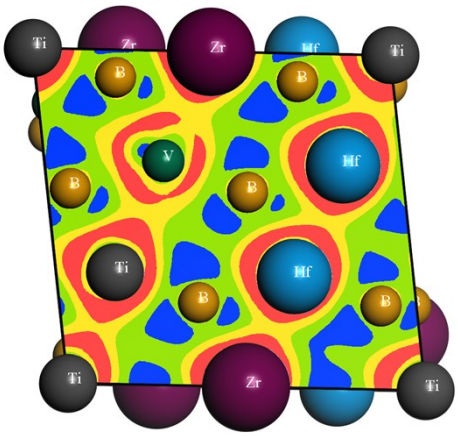
HEB – 9 ($Ti_{0.08}Zr_{0.25}Hf_{0.25}V_{0.42}B$)



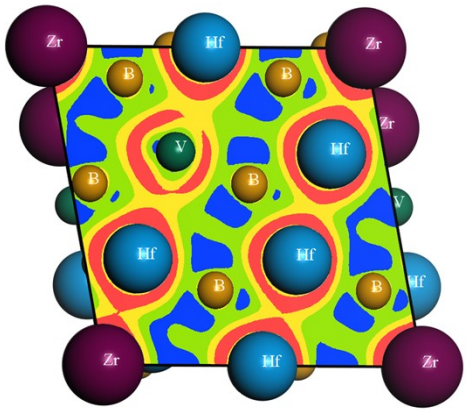
HEB – 10 ($Ti_{0.08}Zr_{0.33}Hf_{0.33}V_{0.25}B$)



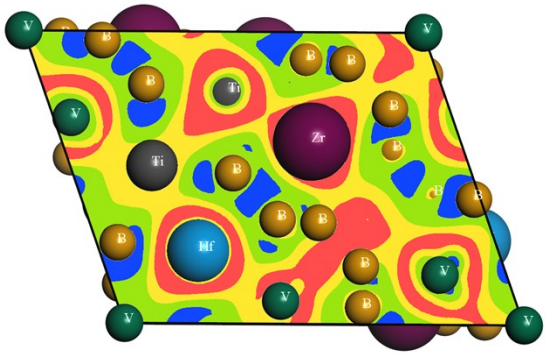
HEB – 11 ($Ti_{0.08}Zr_{0.25}Hf_{0.33}V_{0.33}B$)



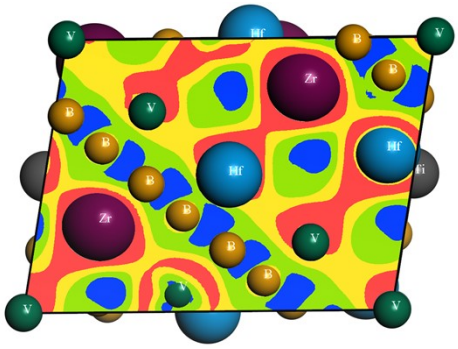
HEB – 12 ($Ti_{0.08}Zr_{0.33}Hf_{0.25}V_{0.33}B$)



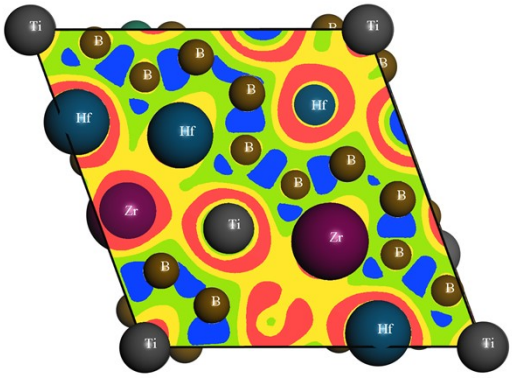
HEB – 13 ($Ti_{0.17}Zr_{0.25}Hf_{0.33}V_{0.25}B$)



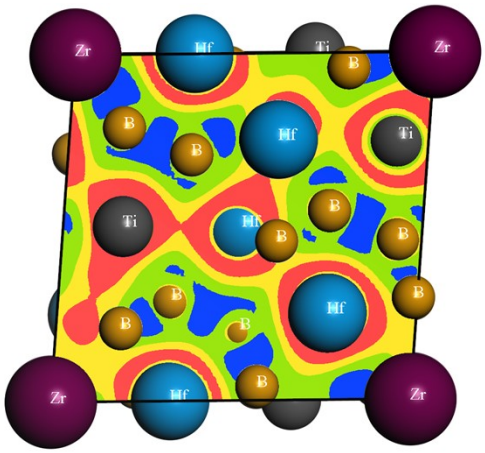
HEB – 14 ($Ti_{0.17}Zr_{0.25}Hf_{0.25}V_{0.33}B$)



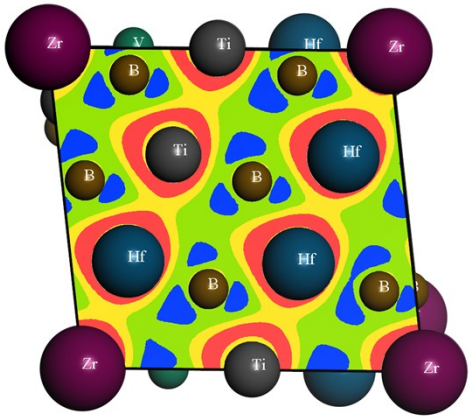
HEB – 15 ($Ti_{0.17}Zr_{0.33}Hf_{0.25}V_{0.25}B$)



HEB - 16 ($Ti_{0.33}Zr_{0.25}Hf_{0.17}V_{0.25}B$)

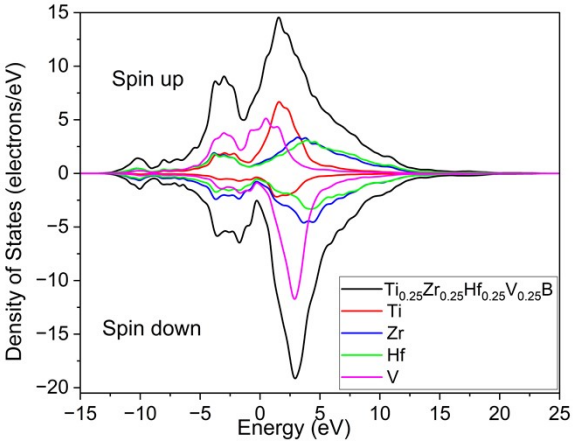


HEB – 17 ($Ti_{0.33}Zr_{0.25}Hf_{0.25}V_{0.17}B$)

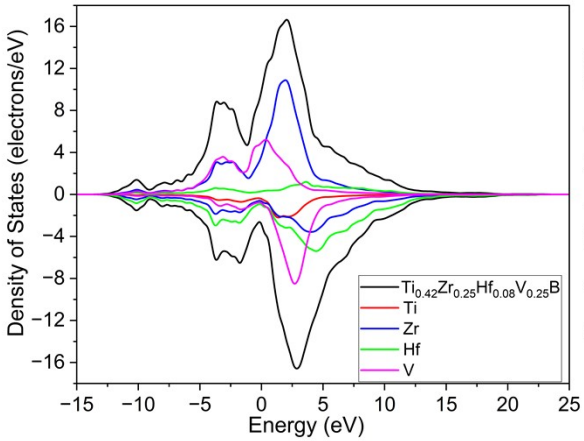


HEB- 18 ($Ti_{0.33}Zr_{0.17}Hf_{0.25}V_{0.25}B$)

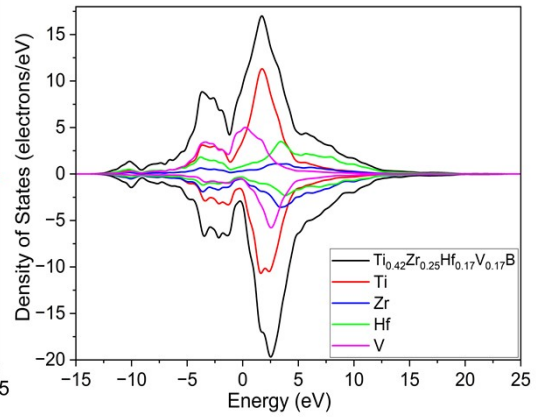
S 7. Spin-up and spin-down total and projected density of states of *d*-orbital of HEBs



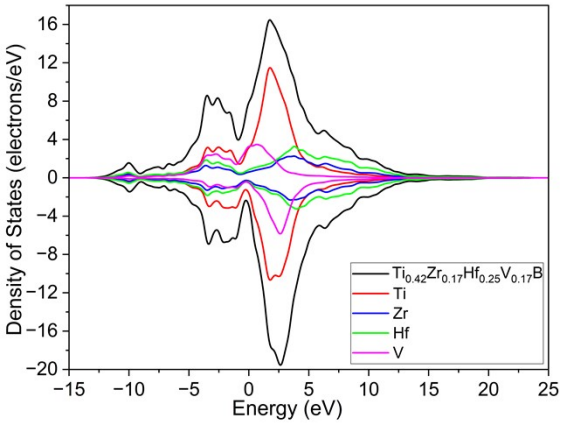
HEB - 1



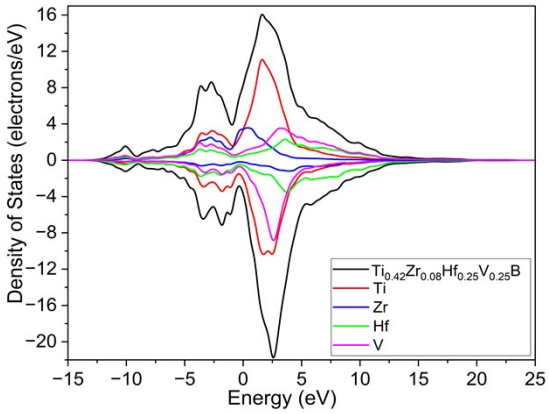
HEB - 2



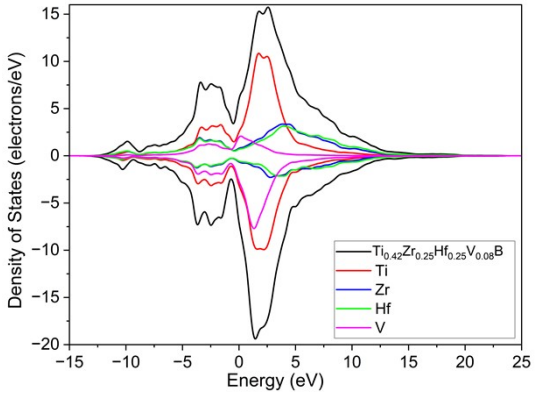
HEB - 3



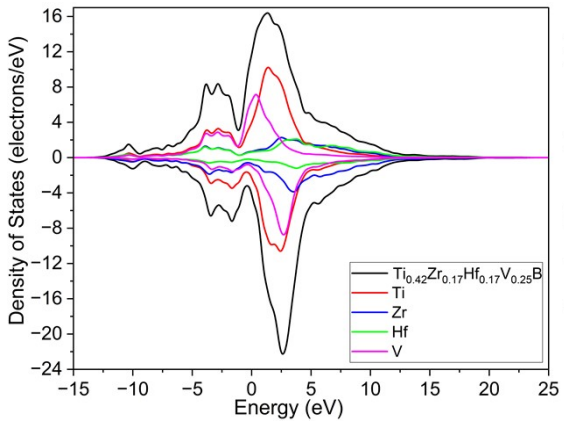
HEB - 4



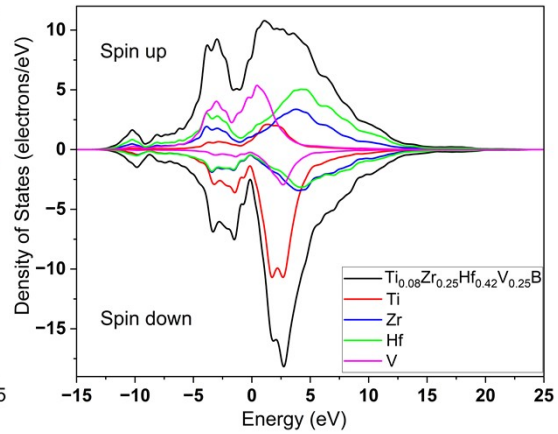
HEB - 5



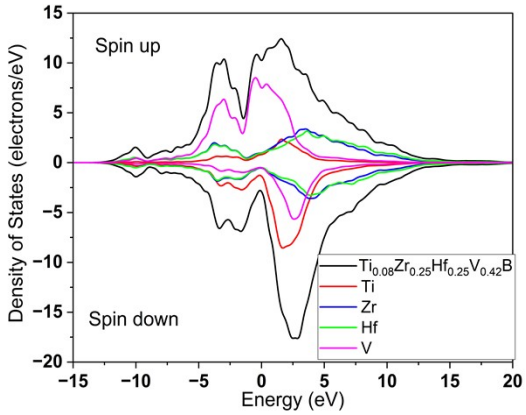
HEB - 6



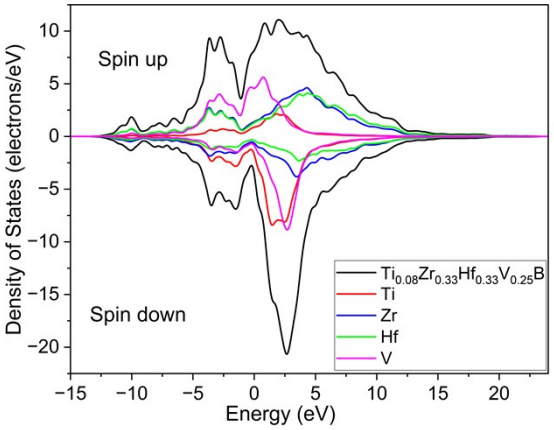
HEB - 7



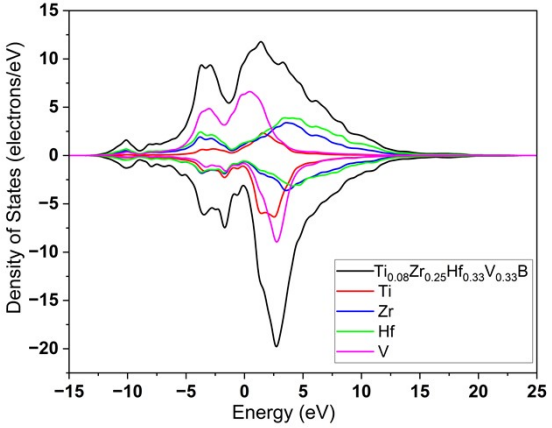
HEB - 8



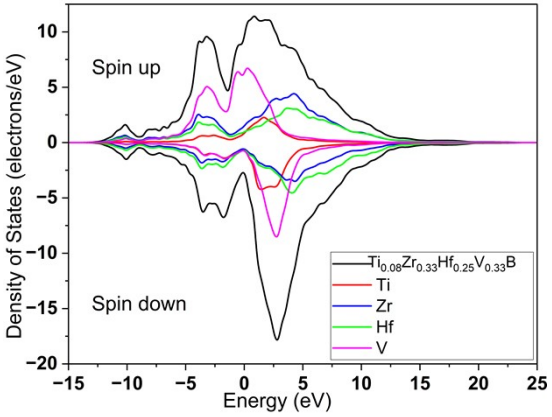
HEB - 9



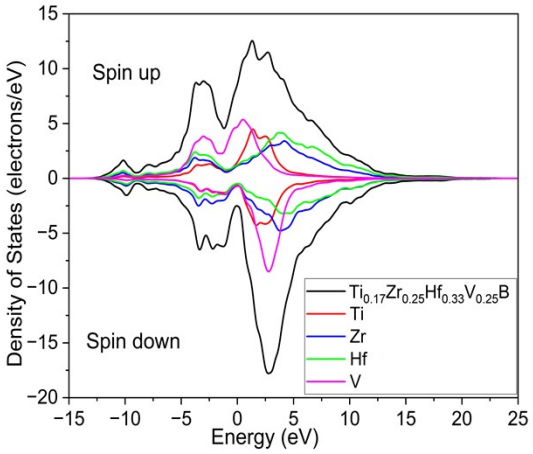
HEB - 10



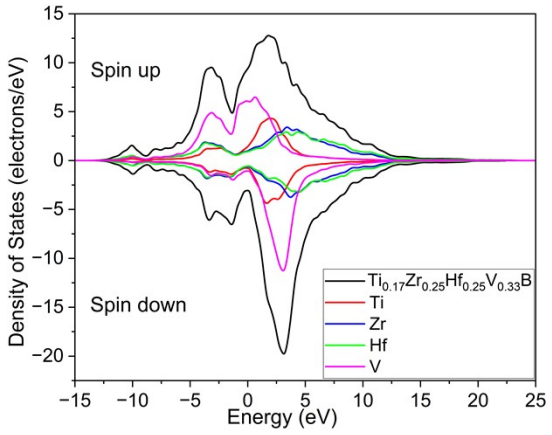
HEB - 11



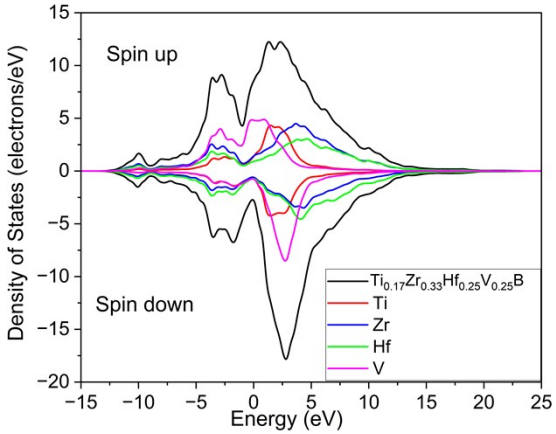
HEB - 12



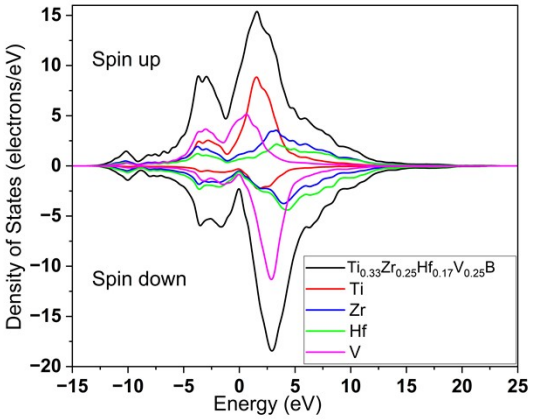
HEB - 13



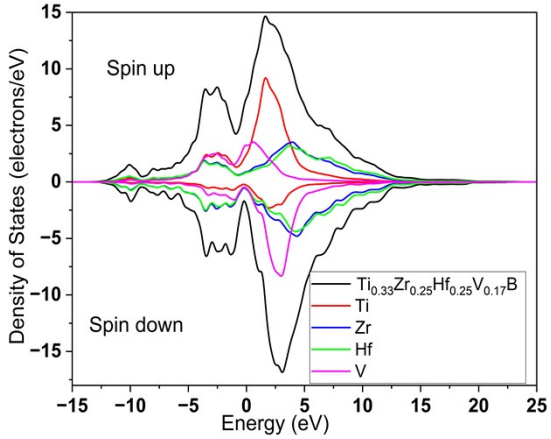
HEB - 14



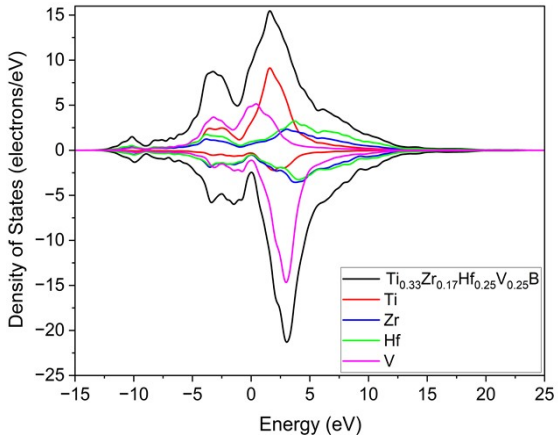
HEB - 15



HEB - 16

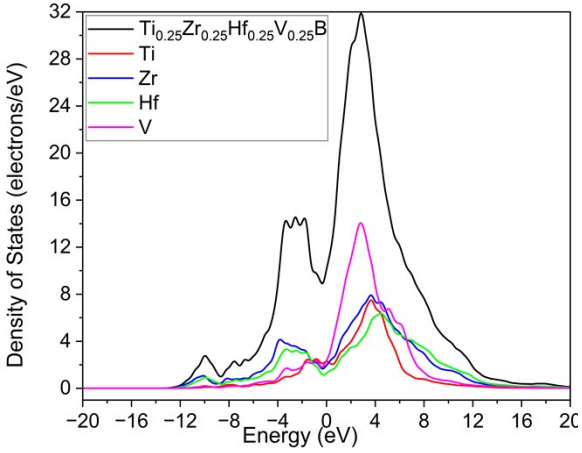


HEB - 17

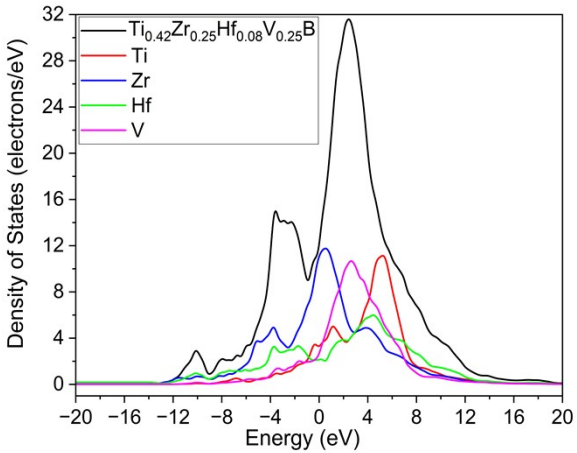


HEB - 18

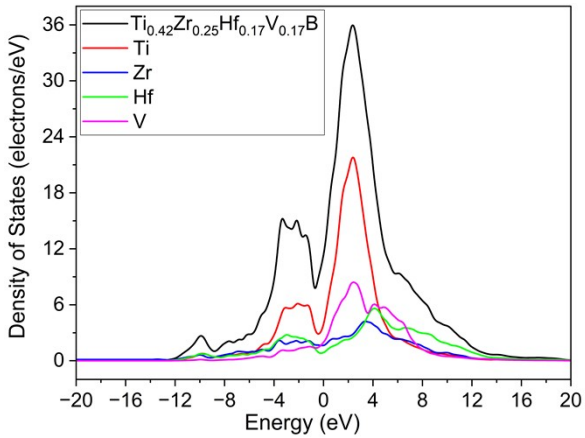
S 8. Overall contribution of partial density of states (PDOS) of *d* orbital's Spin up and Spin down in bonding of all HEBs



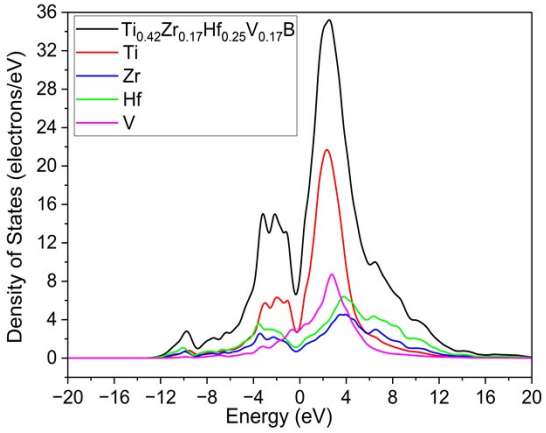
HEB - 1



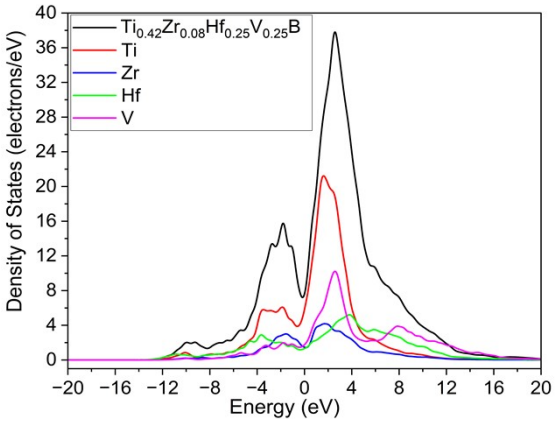
HEB - 2



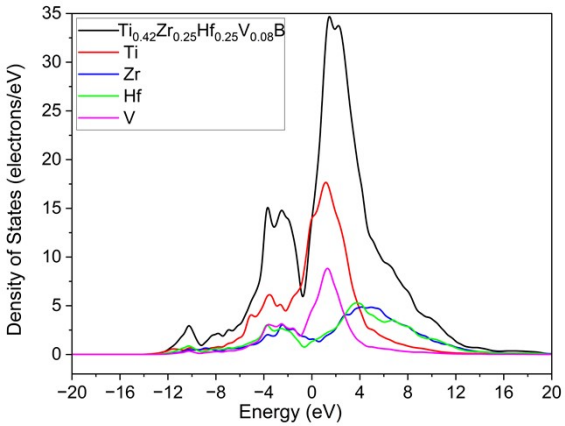
HEB - 3



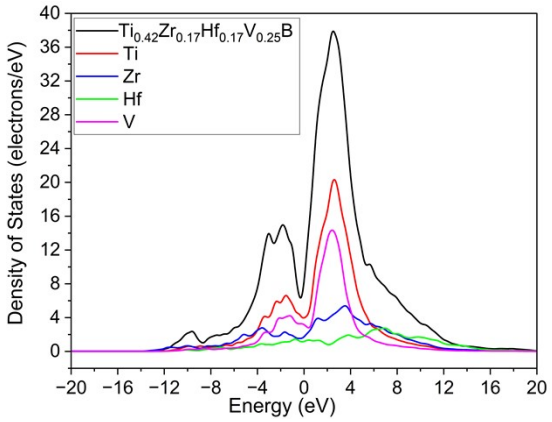
HEB - 4



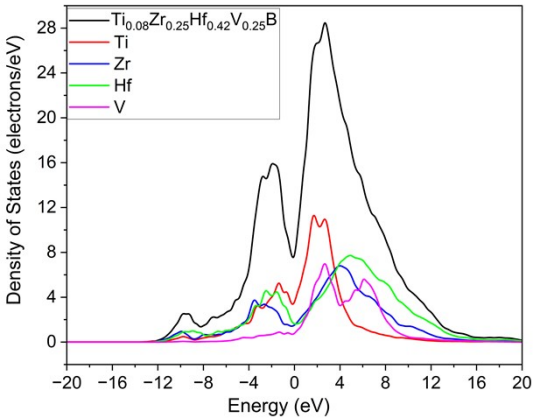
HEB - 5



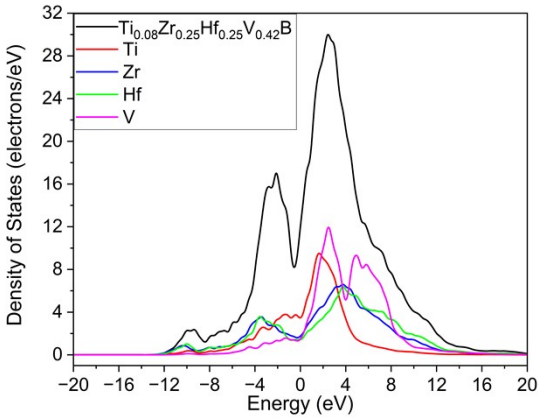
HEB- 6



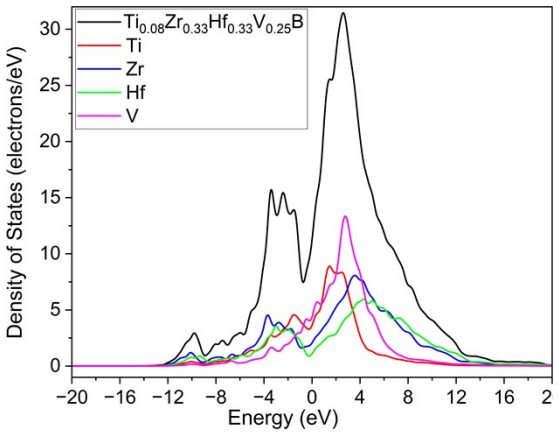
HEB - 7



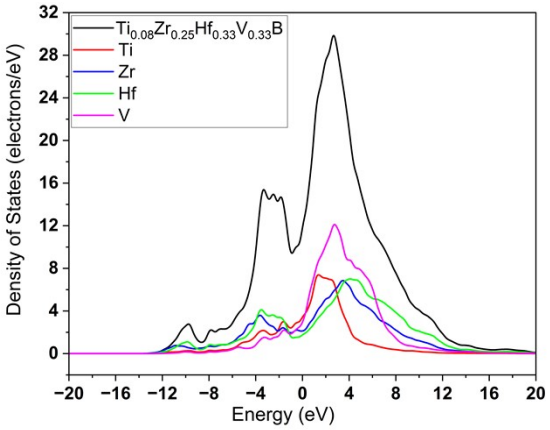
HEB - 8



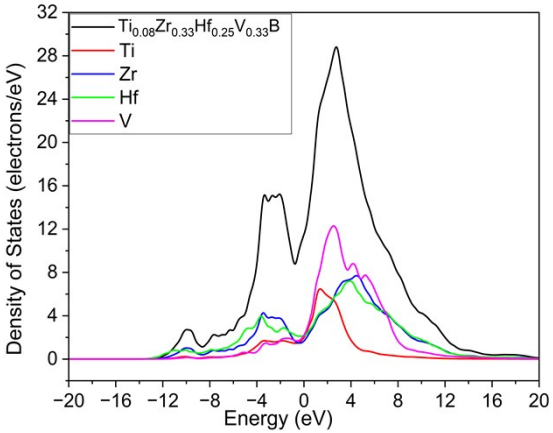
HEB - 9



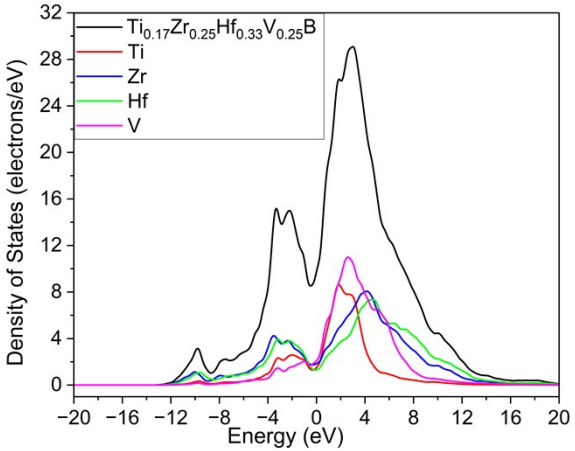
HEB - 10



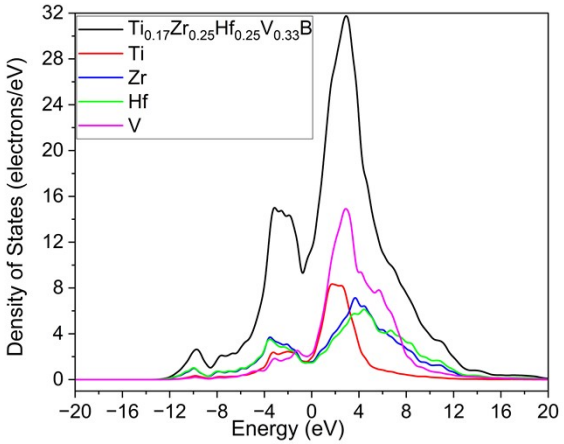
HEB - 11



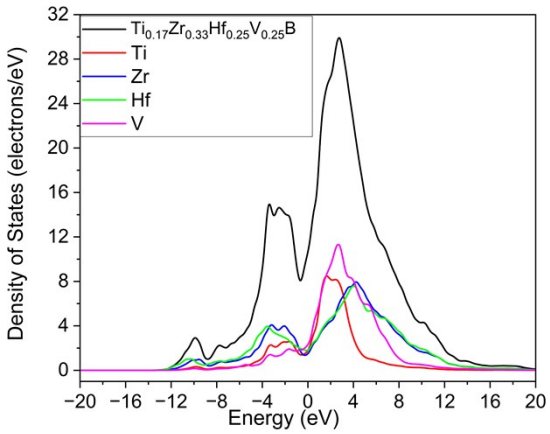
HEB - 12



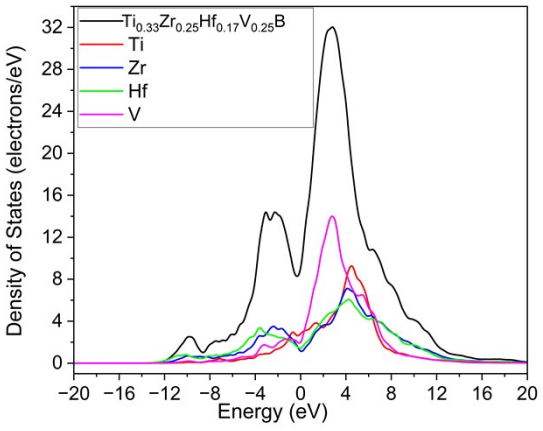
HEB - 13



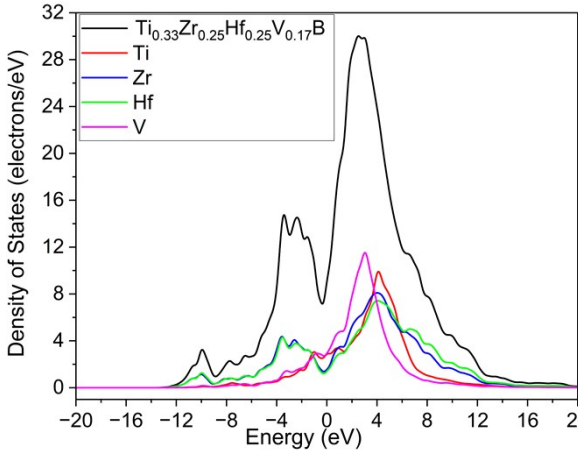
HEB - 14



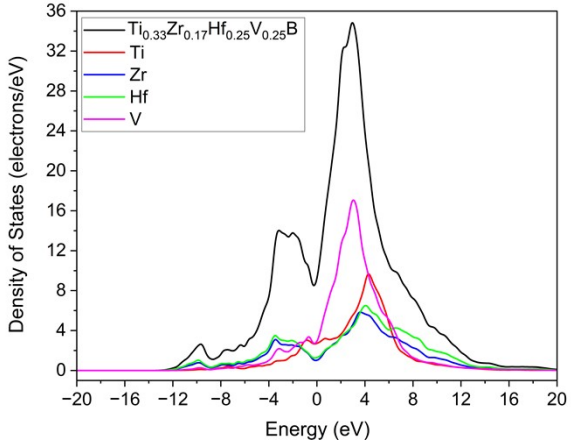
HEB - 15



HEB - 16



HEB - 17



HEB - 18