Supporting information

The structures of W_xN_y crystals and their intrinsic properties: First-principles calculations

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Detailed structure information

1.WxNy(x:y=1:1)

Structure: W_1N_1			
Space group: $P\bar{6}m2$(#187)			
a, b , c	2.84926Å	2.84926Å	2.91404Å
α,β,γ	90°	90°	120°
Wyckoff Position:			
W	0.0000000.0000000.000000		
N	0.333333 0.6666670.500000		

Structure: $W_2N_2(W_4N_4)$			
Space group: *Bm*(#8)			
a, b , c	7.18025Å	2.92240Å	4.27548Å
α,β,γ	90°	101.720°	90°
Wyckoff Position:			
W	0.7292600.5000000.239419		
W	0.8827800.0000000.787540		
N	0.6705970.5000000.714643		
N	0.0028500.5000000.134956		

Structure: $W_3N_3(W_6N_6)$			
Space group: *Pm*3*m*(#221)			
a, b , c	4.11392Å	4.11392Å	4.11392Å
α,β,γ	90°	90°	90°
Wyckoff Position:			
W	0.000000 0.500000 0.000000		
N	0.000000 0.500000 0.500000		

Structure: W_5N_5			
Space group: *P*1(#1)			
a, b , c	4.18776Å	5.14222Å	6.01714Å
α,β,γ	106.438°	89.9987°	65.9794°
Wyckoff Position:			
W	0.0000000.0000000.500000		
W	0.3472330.3054960.811614		
W	0.6399820.7196950.663083		
W	0.3600180.2803050.336917		
W	0.6527670.6945040.188386		
N	0.5000000.0000000.000000		
N	0.8203420.3593160.827345		

N	0.1693030.6610410.661335
N	0.8306970.3389590.338665
N	0.1796580.6406840.172655

2.WxNy(x:y=1:2)

Structure:W_1N_2			
Space group:$P\bar{6}m2$ (#187)			
a, b , c	2.92299Å	2.92299 Å	3.91458 Å
α,β,γ	90º	90º	120º
Wyckoff Position:			
W	0.333333 0.666667 0.500000		
N	0.0000000.0000000.181309		

3.WxNy(x:y=1:3)

Structure:W_1N_3			
Space group:$P\bar{6}m2$ (#187)			
a, b , c	3.41709Å	3.41709 Å	5.17623 Å
α,β,γ	90º	90º	120º
Wyckoff Position:			
W	0.3333330.666667 0.000000		
N	0.0000000.0000000.000000		
N	0.3333330.6666670.612277		

4.WxNy(x:y=1:4)

Structure:W_1N_4			
Space group:*Pmmm* (#47)			
a, b , c	5.13439Å	2.88949Å	4.30217 Å
α,β,γ	90º	90º	90º
Wyckoff Position:			
W	0.5000000.5000000.500000		
N	0.8865750.5000000.500000		
N	0.500000 0.000000 0.856347		

5.WxNy(x:y=1:5)

Structure:W_1N_5			
Space group:*B*2(#5)			
a, b , c	6.08188Å	4.78787Å	5.14451 Å
α,β,γ	90º	91.2388º	90º
Wyckoff Position:			

W	0.0000000.0858730.500000
N	0.5000000.038324 0.500000
N	0.1743200.7061080.499070
N	0.0018950.0842540.887544

6.WxNy(x:y=1:6)

Structure:W_1N_6			
Space group:*P*1(#1)			
a, b , c	3.24155Å	3.23995Å	11.5324 Å
α,β,γ	89.6367^o	89.3922^o	90.0584^o
Wyckoff Position:			
W	0.2760990.8920400.255645		
N	0.2798790.3939130.172159		
N	0.7727160.8901580.339111		
N	0.2291090.3736100.559592		
N	0.1638660.3326060.654015		
N	0.6644060.8312070.855989		
N	0.7450050.8742960.948809		

7.WxNy(x:y=2:1)

Structure:W_2N_1			
Space group:*R*3*m*(#160)			
a, b , c	2.8518Å	2.8518Å	15.6428Å
α,β,γ	90^o	90^o	120^o
Wyckoff Position:			
W	0.000000 0.000000 0.955640		
W	0.000000 0.000000 0.138910		
N	0.000000 0.000000 0.714530		

Structure:W_4N_2			
Space group:*P*6$_3$*/mmc* (#194)			
a, b , c	2.8614Å	2.8614Å	10.3258Å
α,β,γ	90^o	90^o	120^o
Wyckoff Position:			
W	0.666667 0.333333 0.113930		
N	0.333333 0.666667 0.250000		

Structure:W_6N_3			
Space group:*B*2(#5)			
a, b , c	5.1316Å	8.95537Å	5.10987 Å
α,β,γ	90^o	110.568^o	90^o

Wyckoff Position:			
W	0.748907	0.107183	0.734737
W	0.7251220.7787480.726752		
W	0.2610610.9697890.737073		
N	0.500000	0.783608	0.000000
N	0.000000	0.789746	0.500000
N	0.000000	0.937856	0.000000

8.WxNy(x:y=2:3)

Structure:W_2N_3			
Space group:*P*1(#1)			
a, b , c	2.89967Å	3.80213Å	5.57249Å
α,β,γ	79.1640^o	90^o	112.416^o
Wyckoff Position:			
W	0.1557760.6775390.454361		
W	0.8062100.9783380.836477		
N	0.1004710.5668750.843678		
N	0.4212100.2083670.556896		
N	0.7383840.8427300.201758		

Structure:W_4N_6			
Space group:*R*32(#155)			
a, b , c	4.9866Å	4.9866Å	15.7336Å
α,β,γ	90^o	90^o	120^o
Wyckoff Position:			
W	0.000000	0.000000	0.000000
W	0.000000	0.000000	0.176832
W	0.000000	0.000000	0.500000
N	0.970720	0.645790	0.419640

9.WxNy(x:y=2:5)

Structure:W_2N_5			
Space group:*B*2/*m*(#12)			
a, b , c	10.3622Å	3.48609Å	5.05797Å
α,β,γ	90^o	75.6818^o	90^o
Wyckoff Position:			
W	0.1320700.0000000.686650		
N	0.000000	0.000000	0.500000
N	0.000000	0.678519	0.000000
N	0.274845	0.000000	0.307808

10.WxNy(x:y=3:1)

Structure:W_3N_1			
Space group:*Amm*2(#38)			
a, b , c	7.42755Å	3.02443Å	4.69165Å
α,β,γ	90°	90°	90°
Wyckoff Position:			
W	0.805901 0.000000 0.200833		
W	0.500000 0.000000 0.727700		
N	0.000000 0.000000 0.859694		

Structure:W_6N_2			
Space group:*B*2/*b*(#15)			
a, b , c	5.06903Å	8.82035Å	4.91777 Å
α,β,γ	90°	73.1111°	90°
Wyckoff Position:			
W	0.2291320.5901350.492301		
W	0.750000 0.750000 0.500000		
N	0.500000 0.574928 0.750000		

11.WxNy(x:y=3:2)

Structure:W_3N_2			
Space group:$R\bar{3}m$(#166)			
a, b , c	2.8550Å	2.8550Å	24.2117Å
α,β,γ	90°	90°	120°
Wyckoff Position:			
W	0.000000 0.000000 0.381275		
W	0.000000 0.000000 0.500000		
N	0.000000 0.000000 0.772304		

12.WxNy(x:y=3:4)

Structure:W_3N_4			
Space group:*Amm*2(#38)			
a, b , c	2.85946Å	5.57743Å	9.6038Å
α,β,γ	90°	90°	90°
Wyckoff Position:			
W	0.500000 0.000000 0.315280		
W	0.000000 0.000000 0.569490		
W	0.500000 0.000000 0.833750		
N	0.000000 0.7575200.743460		

N	0.500000 0.720980 0.983050

13.WxNy(x:y=3:5)

Structure:W_3N_5			
Space group:*P*1(#1)			
a, b, c	3.79902Å	2.92654Å	7.74022Å
α,β,γ	100.903°	91.7355°	112.661°
Wyckoff Position:			
W	0.2273060.6521150.976829		
W	0.3191010.9952370.571746		
W	0.6779840.5438010.310045		
N	0.9782270.9359650.793821		
N	0.8692030.2349800.501124		
N	0.2579280.8178610.278320		
N	0.5707180.7101890.749929		
N	0.6579620.3990420.039876		

14.WxNy(x:y=4:1)

Structure:W_4N_1			
Space group:*Fmm*2 (#42)			
a, b, c	3.08368Å	19.2066Å	4.63895Å
α,β,γ	90°	90°	90°
Wyckoff Position:			
W	0.000000 0.1913910.971459		
W	0.000000 0.074950 0.445996		
N	0.500000 0.500000 0.103019		

15.WxNy(x:y=4:3)

Structure:W_4N_3			
Spacegroup:*P*1(#1)			
a, b, c	2.91183Å	4.12121Å	7.67648Å
α,β,γ	74.4340°	100.613°	89.9949°
Wyckoff Position:			
W	0.6960910.2994670.900991		
W	0.1011390.8982460.703709		
W	0.8988610.1017540.296291		
W	0.3039090.7005330.099009		
N	0.1003410.3984600.703175		
N	0.500000 0.000000 0.500000		
N	0.8996590.601540 0.296825		

16.WxNy(x:y=4:5)

Structure: W_4N_5			
Space group: $B2$(#5)			
a, b, c	6.19807Å	4.94077Å	6.29911Å
α,β,γ	90°	91.6205°	90°
Wyckoff Position:			
W	0.299131	0.603433	0.391887
W	0.114420	0.606034	0.810181
N	0.314080	0.260402	0.893769
N	0.102041	0.269917	0.305328
N	0.500000	0.271037	0.500000

17.WxNy(x:y=5:1)

Structure: W_5N_1			
Space group: $B2/m$(#12)			
a, b, c	14.0786Å	4.36430Å	2.77153Å
α,β,γ	90°	90.354°	90°
Wyckoff Position:			
W	0.701793	0.500000	0.829296
W	0.000000	0.000000	0.000000
W	0.885659	0.500000	0.506712
N	0.000000	0.500000	0.000000

18.WxNy(x:y=5:2)

Structure: W_5N_2			
Space group: $B2/m$(#12)			
a, b, c	9.014Å	4.21907Å	6.60207Å
α,β,γ	90°	134.654°	90°
Wyckoff Position:			
W	0.925500	0.500000	0.619250
W	0.000000	0.000000	0.000000
W	0.716570	0.500000	0.820620
N	0.605040	0.500000	0.408350

19.WxNy(x:y=5:3)

Structure: W_5N_3			
Space group: $P1$(#1)			
a, b, c	2.87395Å	5.33390Å	6.56185Å

α,β,γ	95.03868°	102.58678°	90.14283°
Wyckoff Position:			
W	0.465487	0.091867	0.146000
W	0.724015	0.438835	0.656502
W	0.401955	0.585840	0.014125
W	0.773807	0.928187	0.762272
W	0.084699	0.743368	0.383346
N	0.623048	0.033587	0.457770
N	0.988290	0.399275	0.190542
N	0.304899	0.228611	0.822272

20.WxNy(x:y=5:4)

Structure:W_5N_4			
Space group:*P*1(#1)			
a, b , c	15.32492Å	2.96084Å	8.07548Å
α,β,γ	90°	143.85284°	90°
Wyckoff Position:			
W	0.345960	0.500000	0.004151
W	0.328122	0.500000	0.491455
W	0.154040	0.000000	0.995849
W	0.171878	0.000000	0.508545
W	0.000000	0.500000	0.000000
W	0.845960	0.000000	0.004151
W	0.828122	0.000000	0.491455
W	0.654040	0.500000	0.995849
W	0.671878	0.500000	0.508545
W	0.500000	0.000000	0.000000
N	0.190125	0.000000	0.789941
N	0.010566	0.500000	0.287001
N	0.989434	0.500000	0.712999
N	0.309875	0.500000	0.210059
N	0.690125	0.500000	0.789941
N	0.510566	0.000000	0.287001
N	0.489434	0.000000	0.712999
N	0.809875	0.000000	0.210059

21.WxNy(x:y=5:6)

Structure:W_5N_4			
Space group:$P\bar{6}2m$(#189)			
a, b , c	4.89641Å	4.89641Å	5.63848Å
α,β,γ	90°	90°	120°

Wyckoff Position:			
W	0.666667	0.333333	0.500000
W	0.000000	0.000000	0.500000
W	0.333333	0.666667	0.000000
N	0.335269	0.000000	0.740504

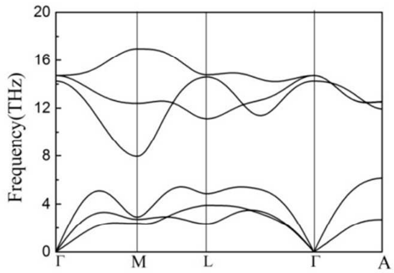
22.WxNy(x:y=6:1)

Structure: W_5N_4			
Space group: *P*2/*m*(#10)			
a, b, c	2.76723Å	4.36680Å	8.41747Å
α,β,γ	90°	83.8561°	90°
Wyckoff Position:			
W	0.429093	0.000000	0.692368
W	0.000000	0.500000	0.500000
W	0.279904	0.500000	0.156584
W	0.000000	0.000000	0.000000
N	0.000000	0.000000	0.500000

23.WxNy(x:y=6:5)

Structure: W_6N_5			
Space group: C 2/m (#12)			
a, b, c	9.29200Å	4.16984Å	6.65809Å
α,β,γ	90°	99.2203°	90°
Wyckoff Position:			
W	0.148044	0.000000	0.427490
W	0.796110	0.500000	0.836370
W	0.941619	0.500000	0.301378
N	0.777269	0.000000	0.863449
N	0.066938	0.000000	0.714593
N	0.000000	0.500000	0.000000

Phonon spectra



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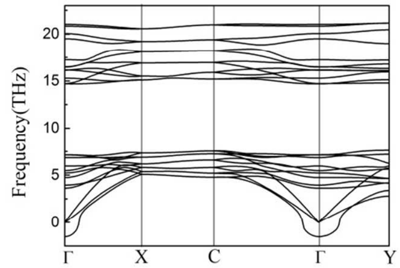

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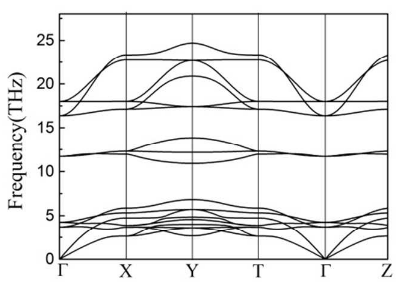

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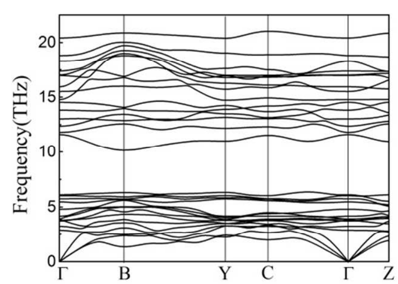

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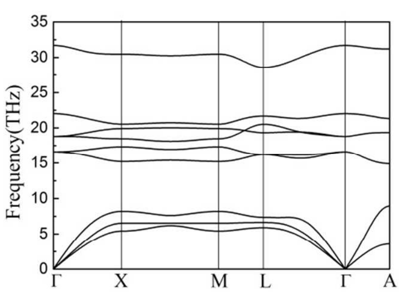

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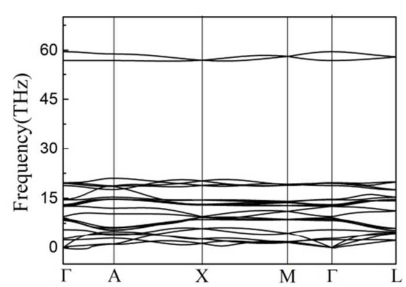

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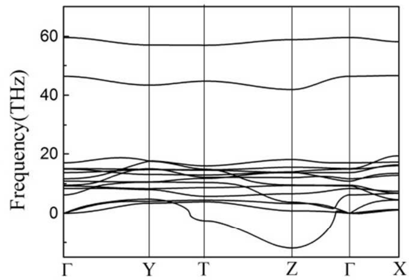

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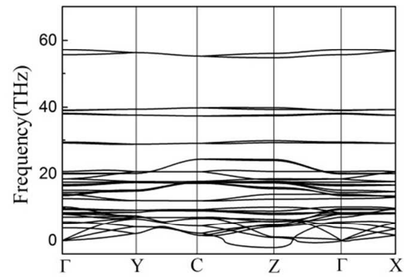

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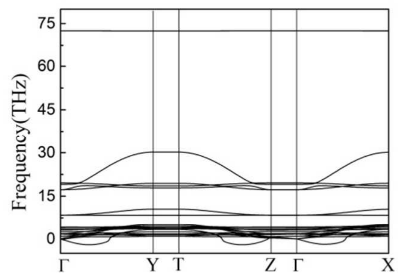

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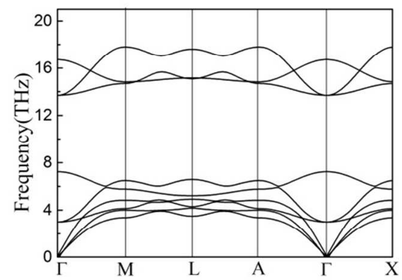

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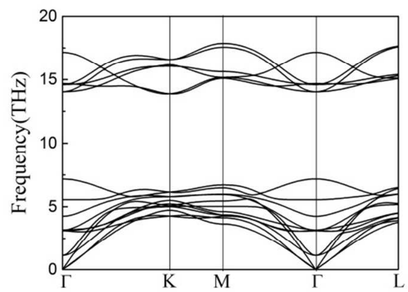
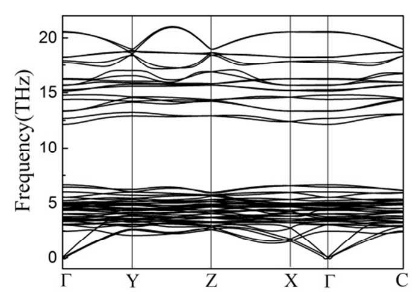


W_4N_2



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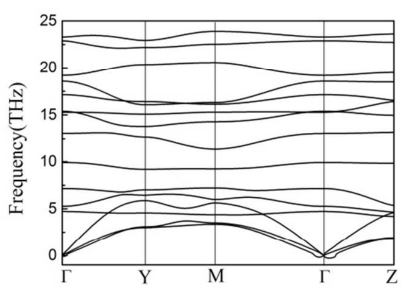

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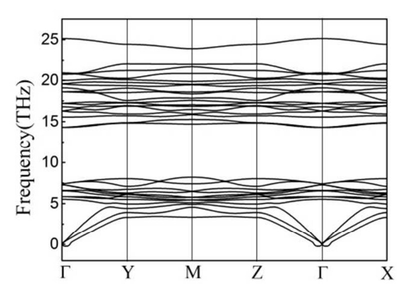

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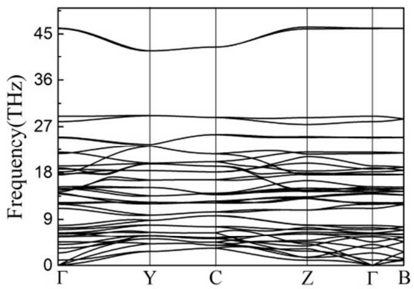

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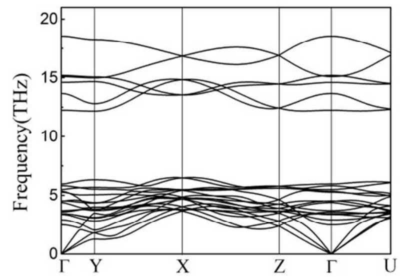

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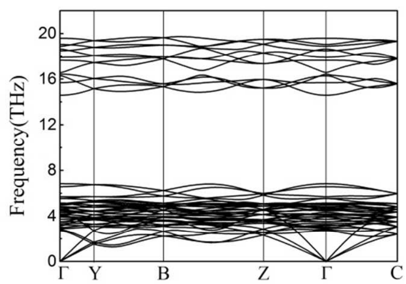

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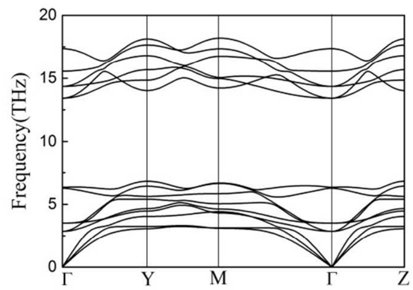

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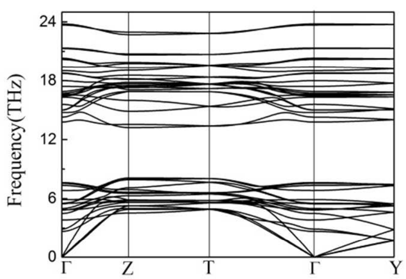

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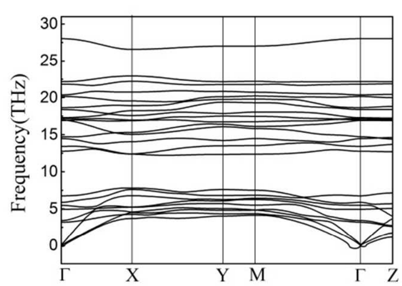

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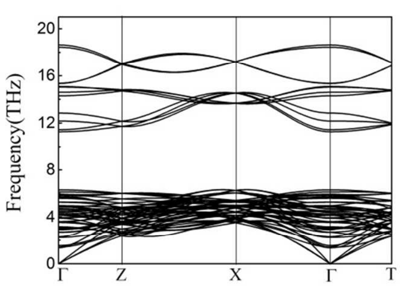

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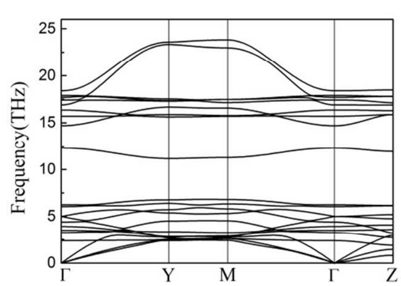

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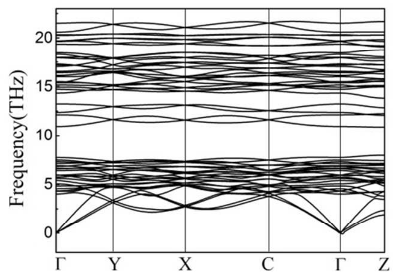
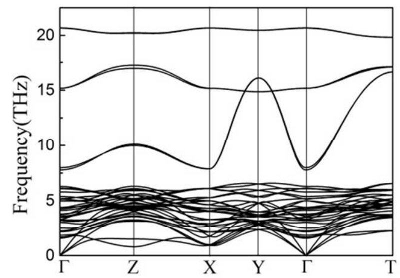
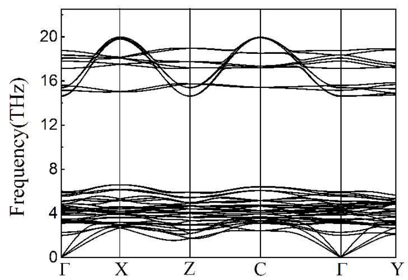


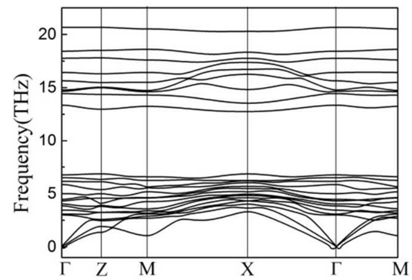
W_4N_5



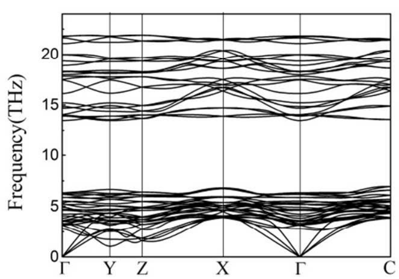
W_5N_1



W_5N_2



W_5N_3



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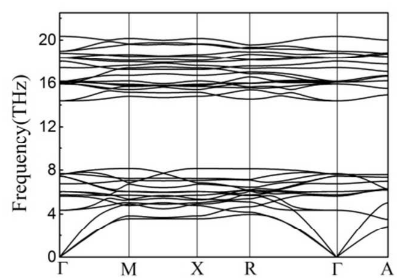
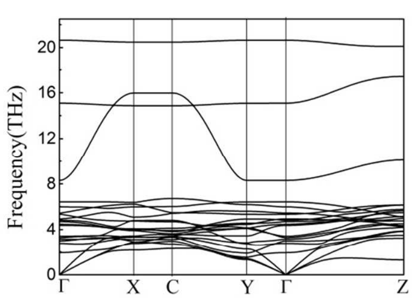
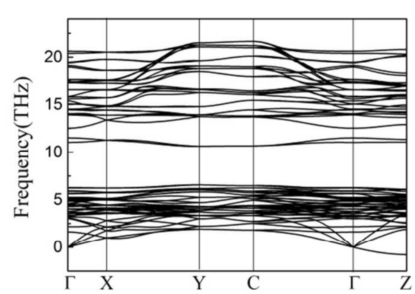


W_5N_6

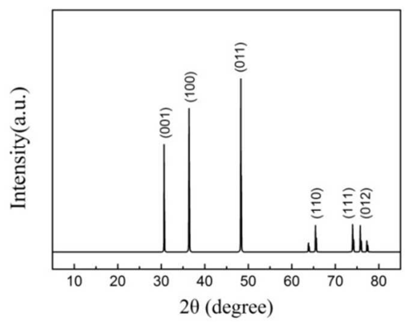


W_6N_1

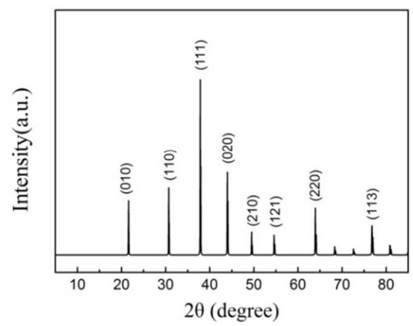


W_6N_5

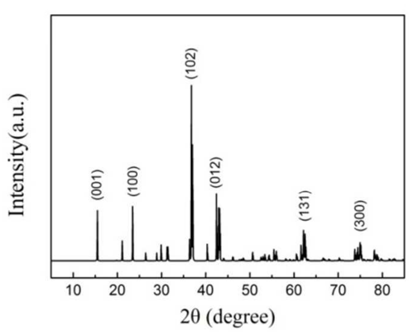
XRD spectra



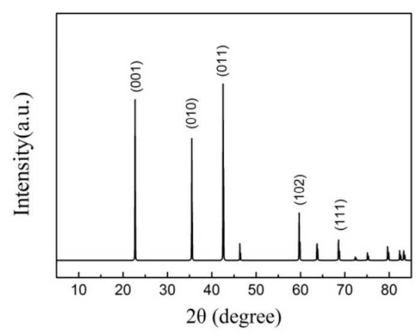
W_1N_1



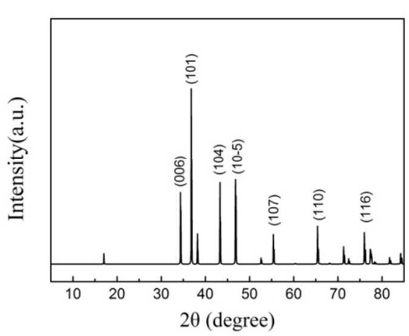
W_3N_3



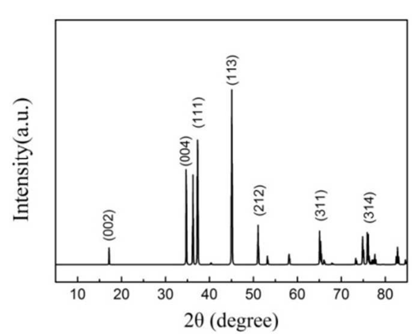
W_5N_5



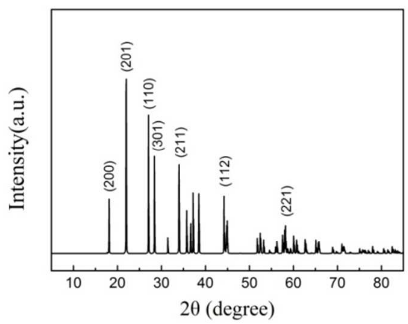
W_1N_2



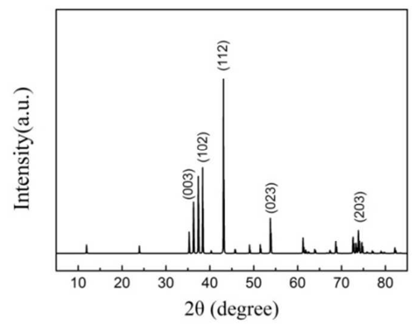
W_2N_1



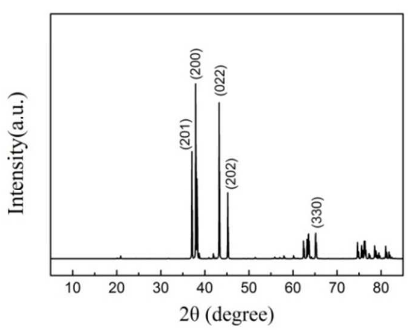
W_4N_2



W_2N_5



W_3N_1



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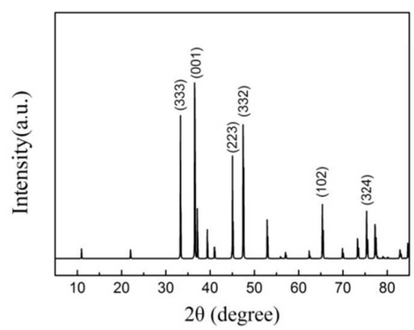

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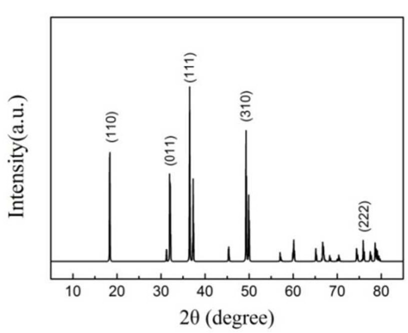
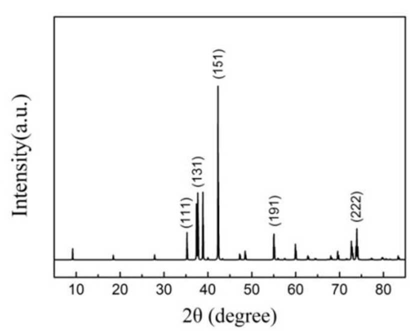
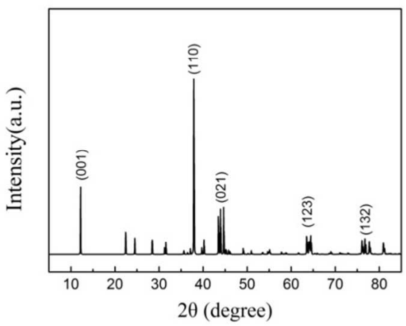


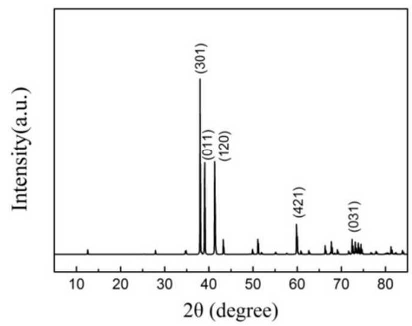
W_3N_4



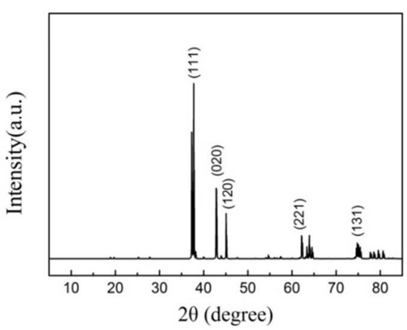
W_4N_1



W_4N_3



W_5N_1



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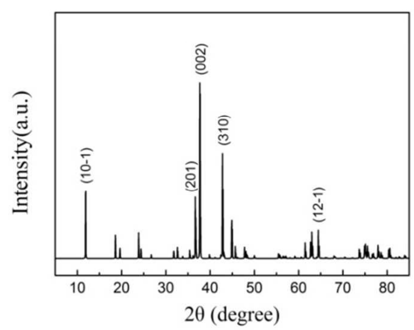

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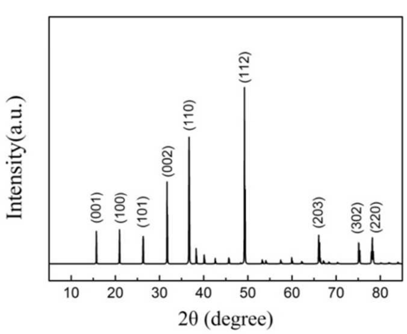
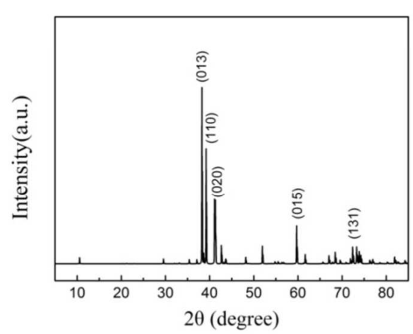
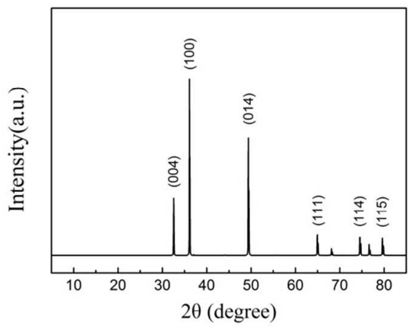


W_5N_6



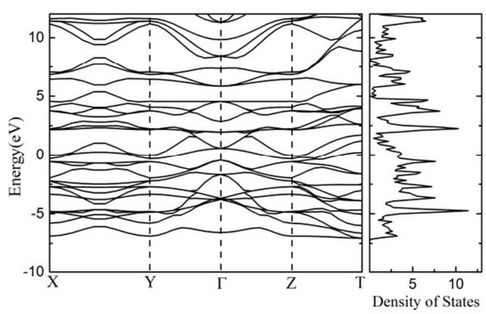
W_6N_1



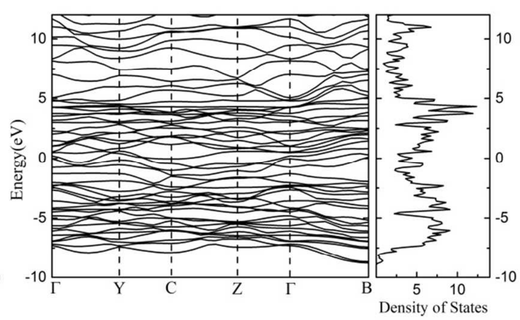
$W_4N_{4\text{-exp-2}}$

Band structures and the DOS

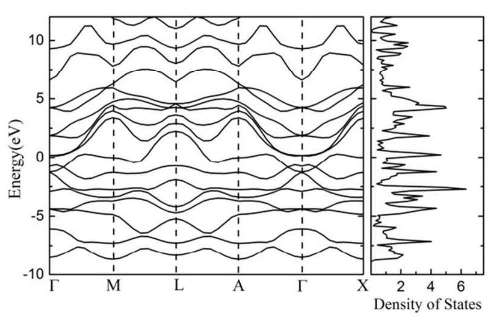
Here, the Fermi energy levels are all at 0.0 eV.



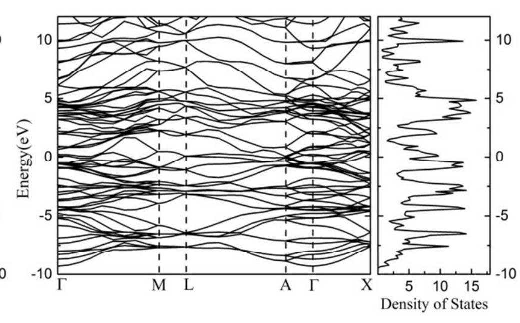
W_3N_3



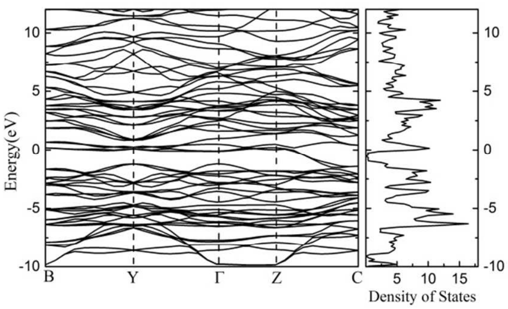
W_5N_5



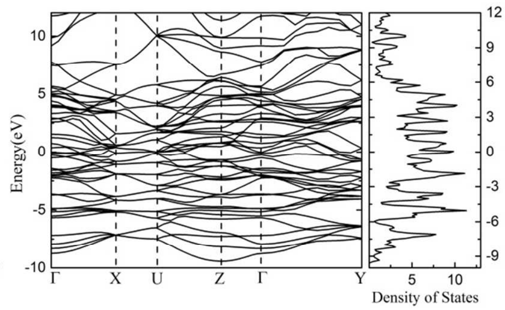
W_2N_1



W_4N_2



W_2N_5



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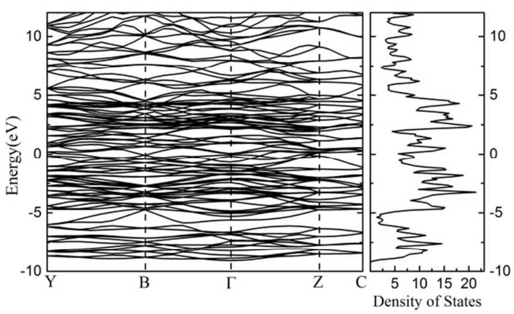

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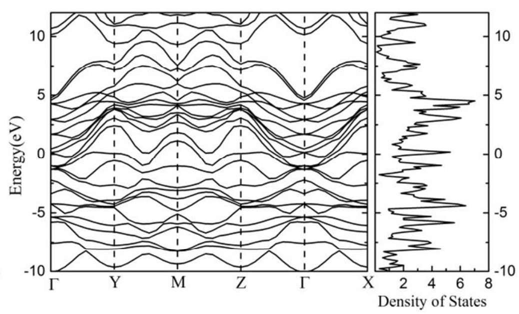
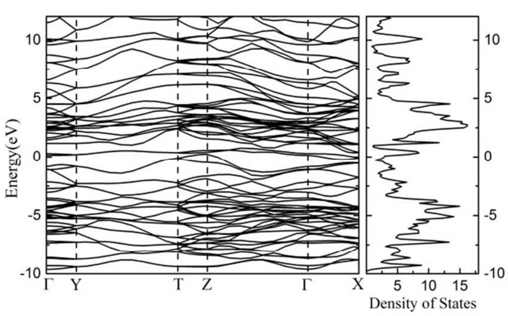
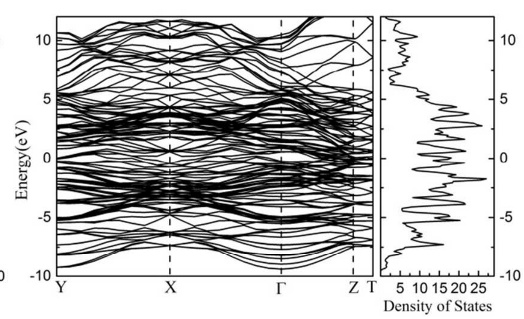


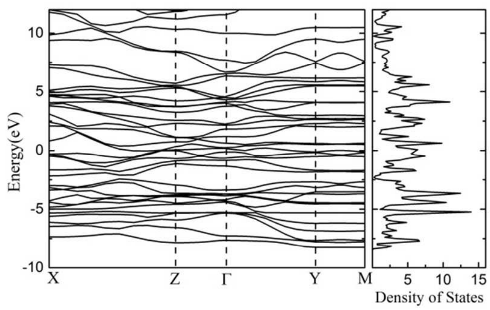
W_3N_2



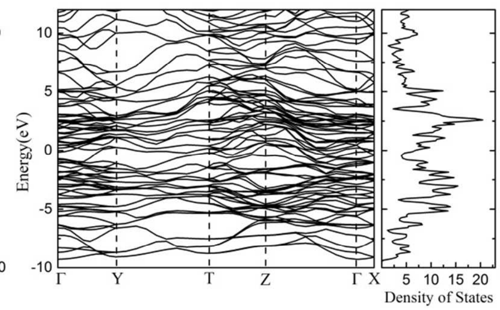
W_3N_4



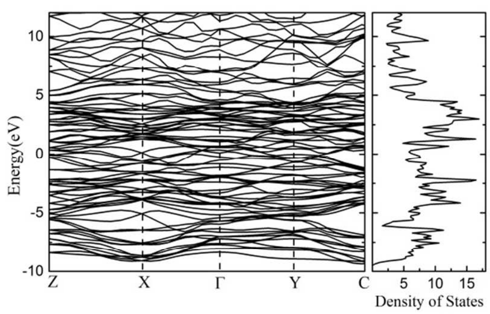
W_4N_1



W_4N_3



W_5N_1



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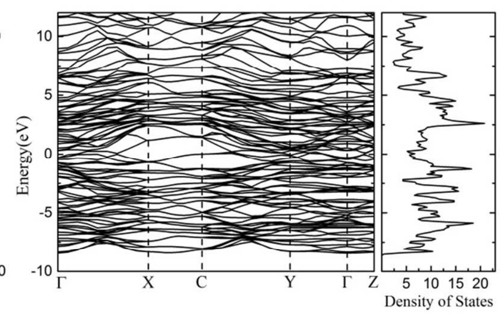

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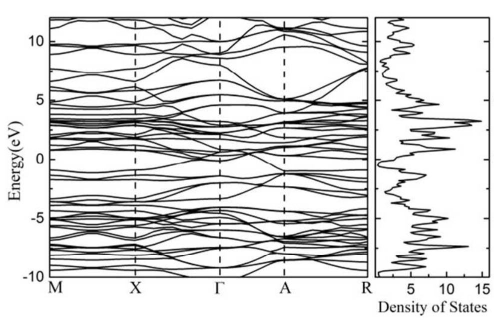
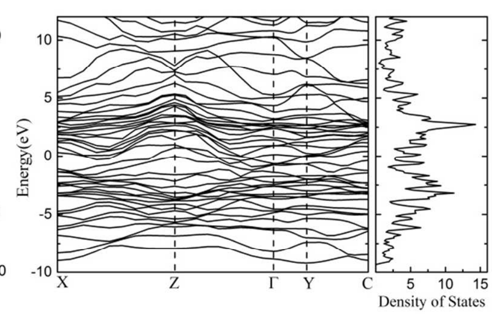
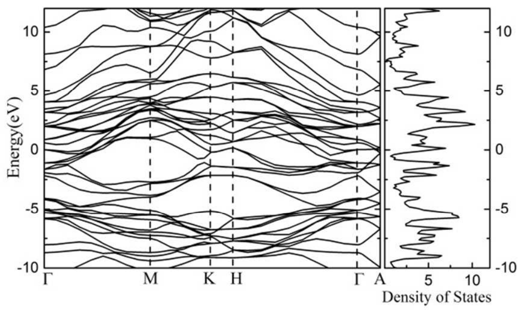


W_5N_6



W_6N_1



$W_4N_{4\text{-exp-2}}$