

## Supplementary Information File

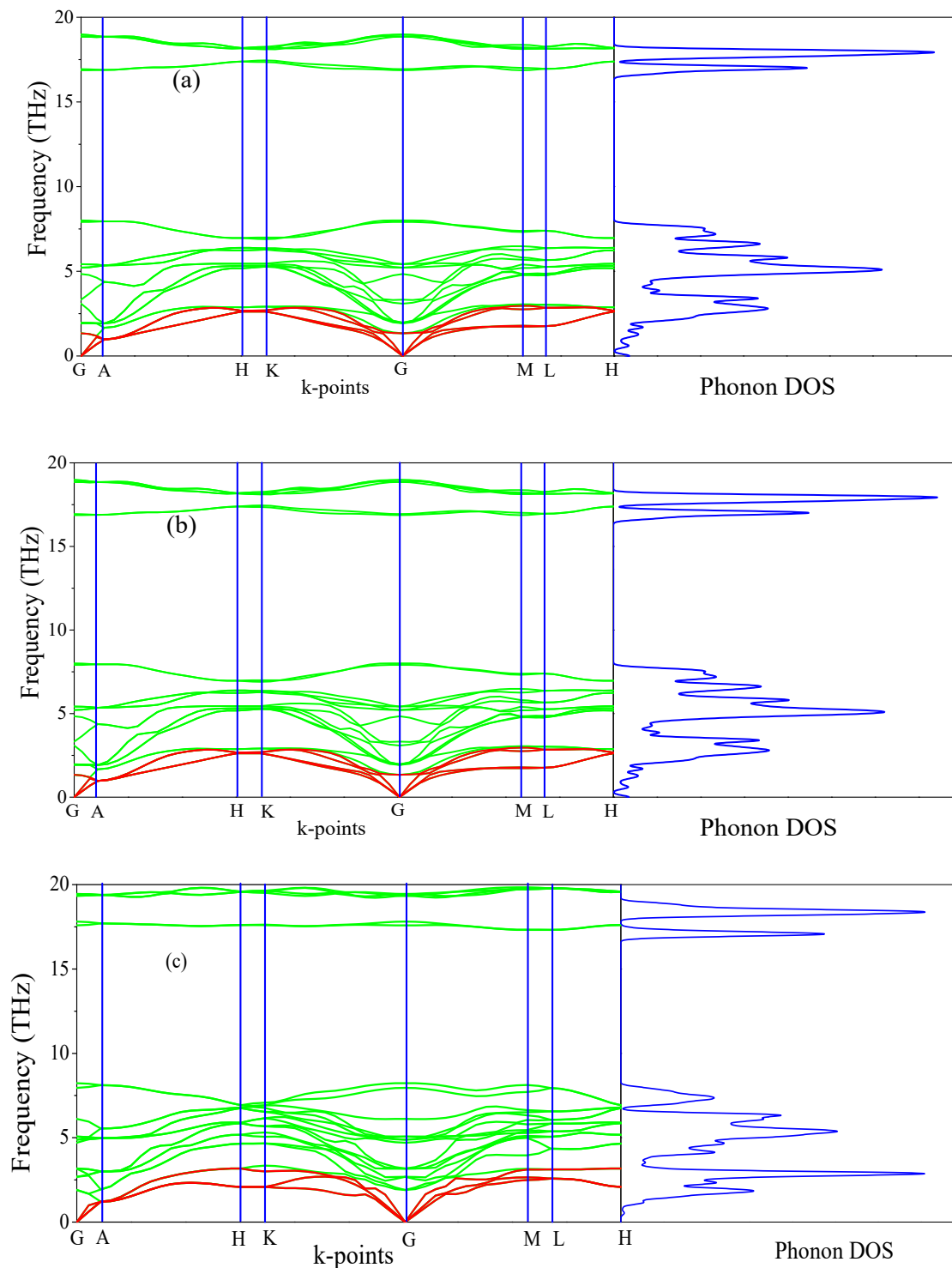
### DFT insights into Nb-based 211 MAX phase carbides:

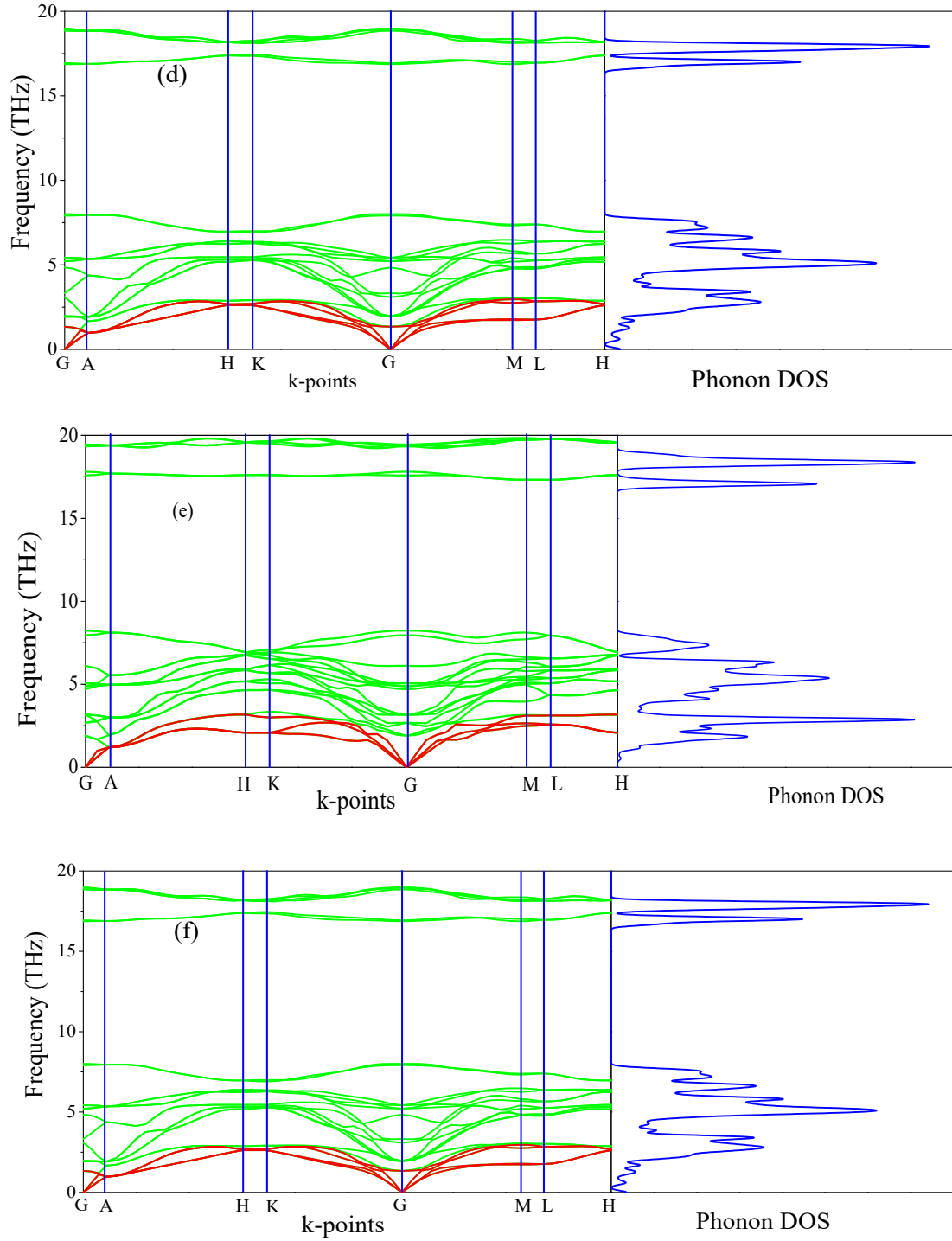
#### $\text{Nb}_2\text{AC}$ (A= Ga, Ge, Tl, Zn, P, In, Cd)

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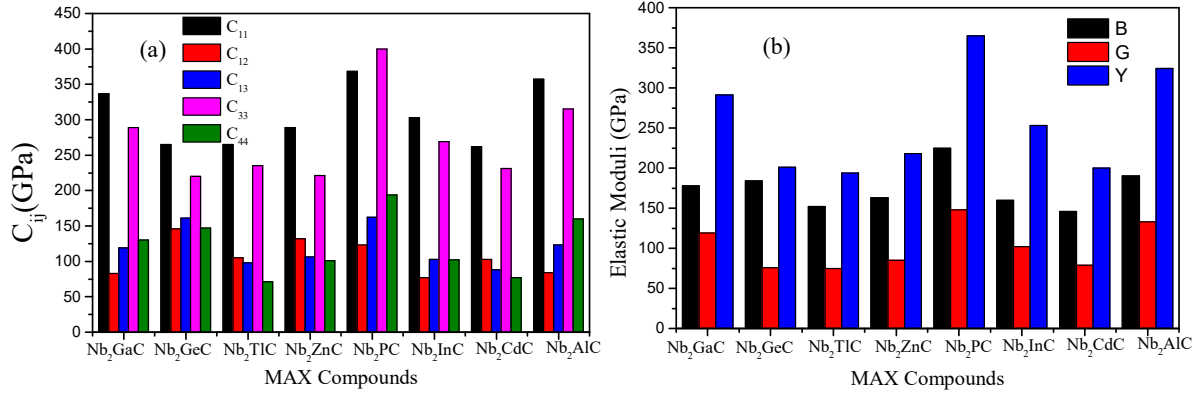
Chattogram-4349, Bangladesh



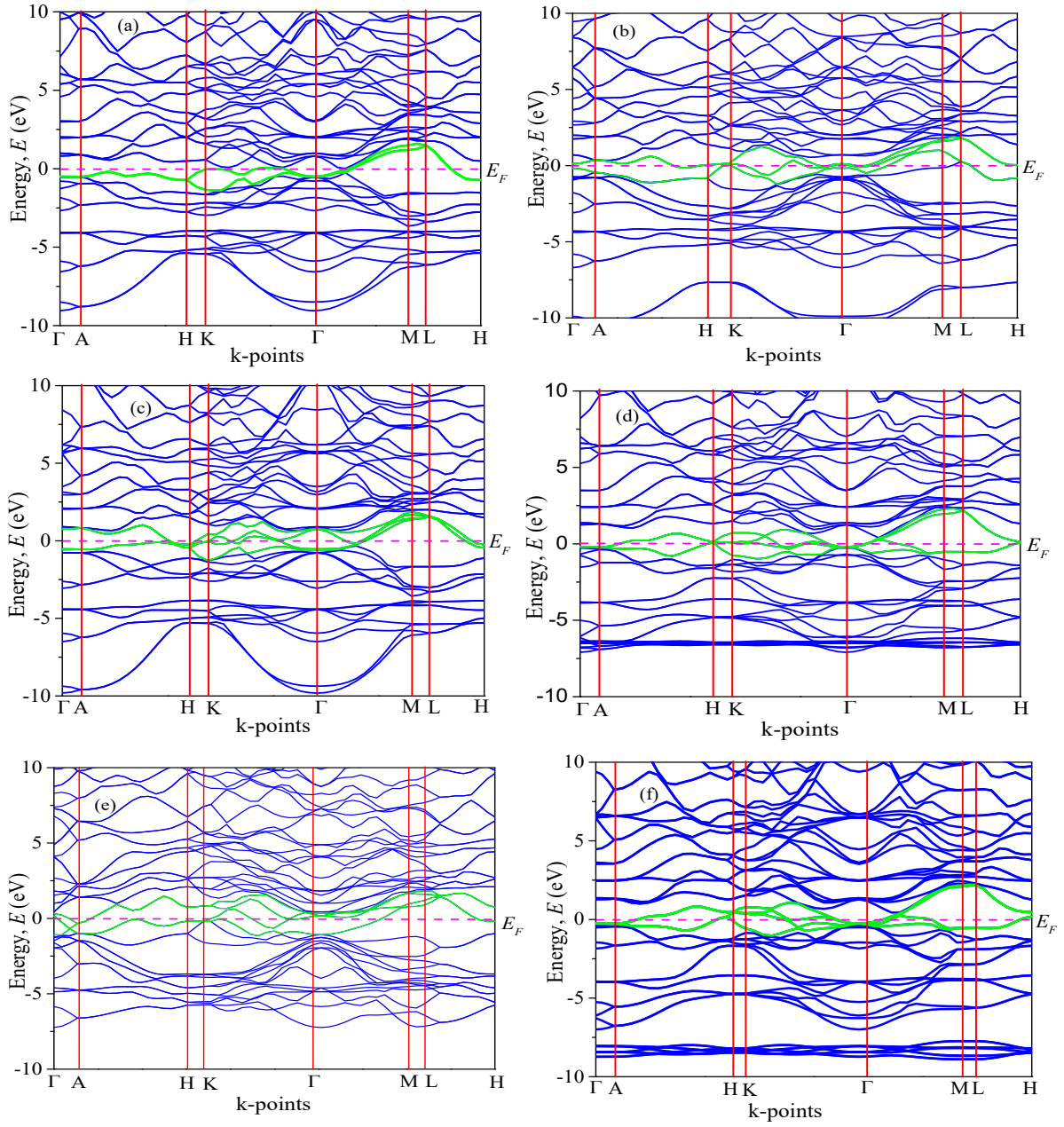


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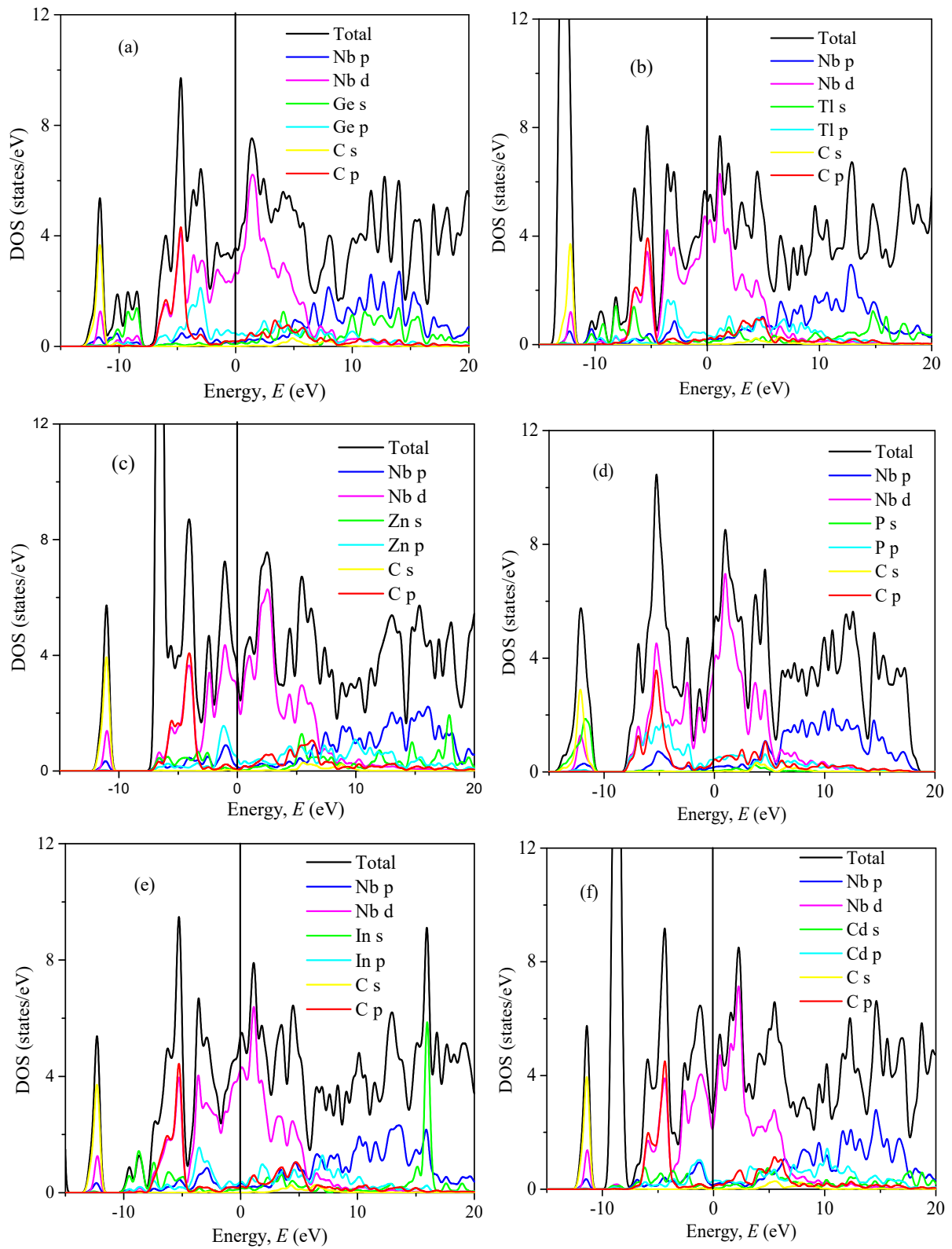
**Fig.S-1:** Phonon dispersion curve and phonon DOS of (a) Nb<sub>2</sub>GeC, (b) Nb<sub>2</sub>TlC, (c) Nb<sub>2</sub>ZnC, (d) Nb<sub>2</sub>PC, (e) Nb<sub>2</sub>InC and (f) Nb<sub>2</sub>CdC calculated using GGA PBEsol.



**Fig.S-2:** (a) The stiffness constant and (b) elastic moduli of Nb<sub>2</sub>AC (A = Ga, Ge, Ti, Zn, P, In, Cd, Al) MAX phases calculated using GGA PBE.

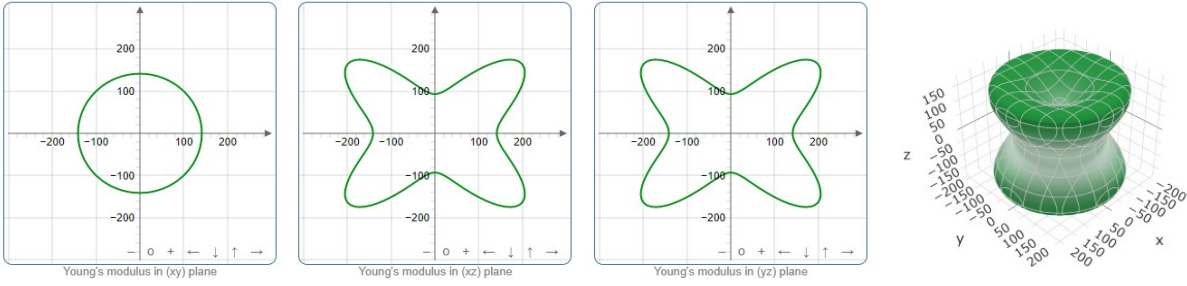


**Fig.S-3:** Band Structure of a)  $\text{Nb}_2\text{GeC}$ , b)  $\text{Nb}_2\text{TlC}$ , c)  $\text{Nb}_2\text{ZnC}$ , d)  $\text{Nb}_2\text{PC}$ , e)  $\text{Nb}_2\text{ZnC}$  and f)  $\text{Nb}_2\text{CdC}$  calculated using GGA PBEsol.

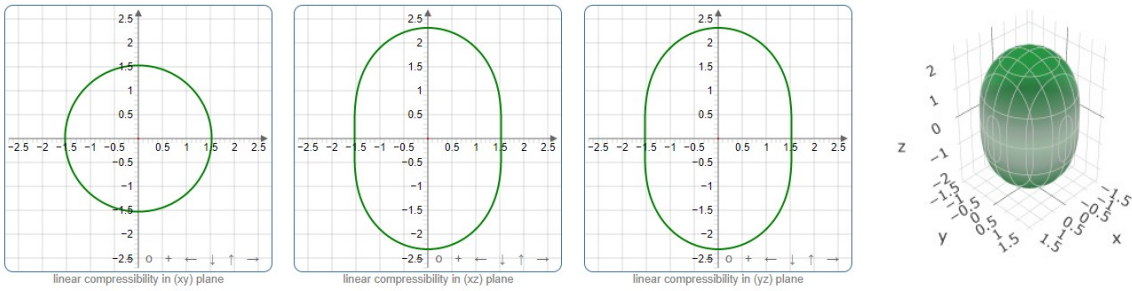


**Fig.S-4:** Total and Partial DOS of a) Nb<sub>2</sub>GeC, b) Nb<sub>2</sub>TiC, c) Nb<sub>2</sub>ZnC, d) Nb<sub>2</sub>PC, e) Nb<sub>2</sub>ZnC and f) Nb<sub>2</sub>CdC calculated using GGA PBEsol.

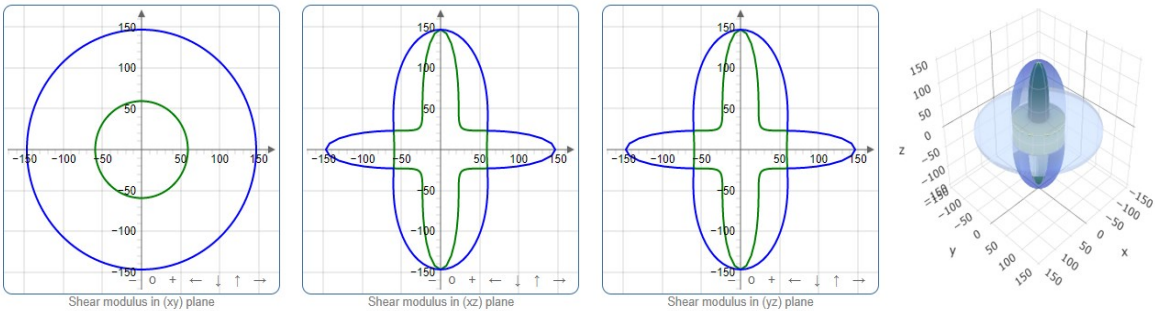
**(a) Young's modulus**



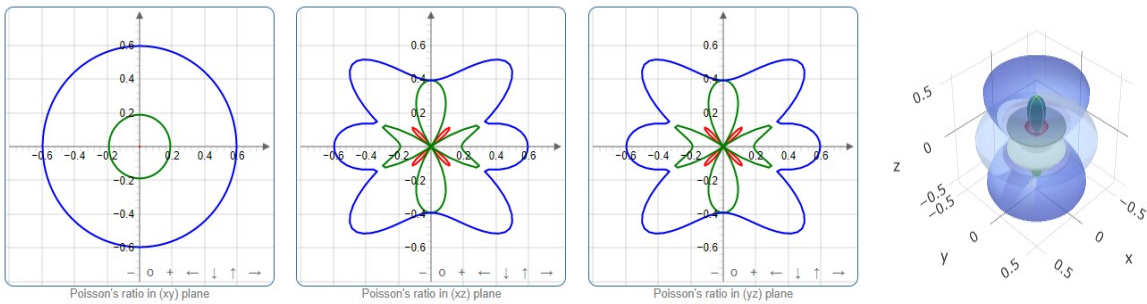
**(b) Compressibility**



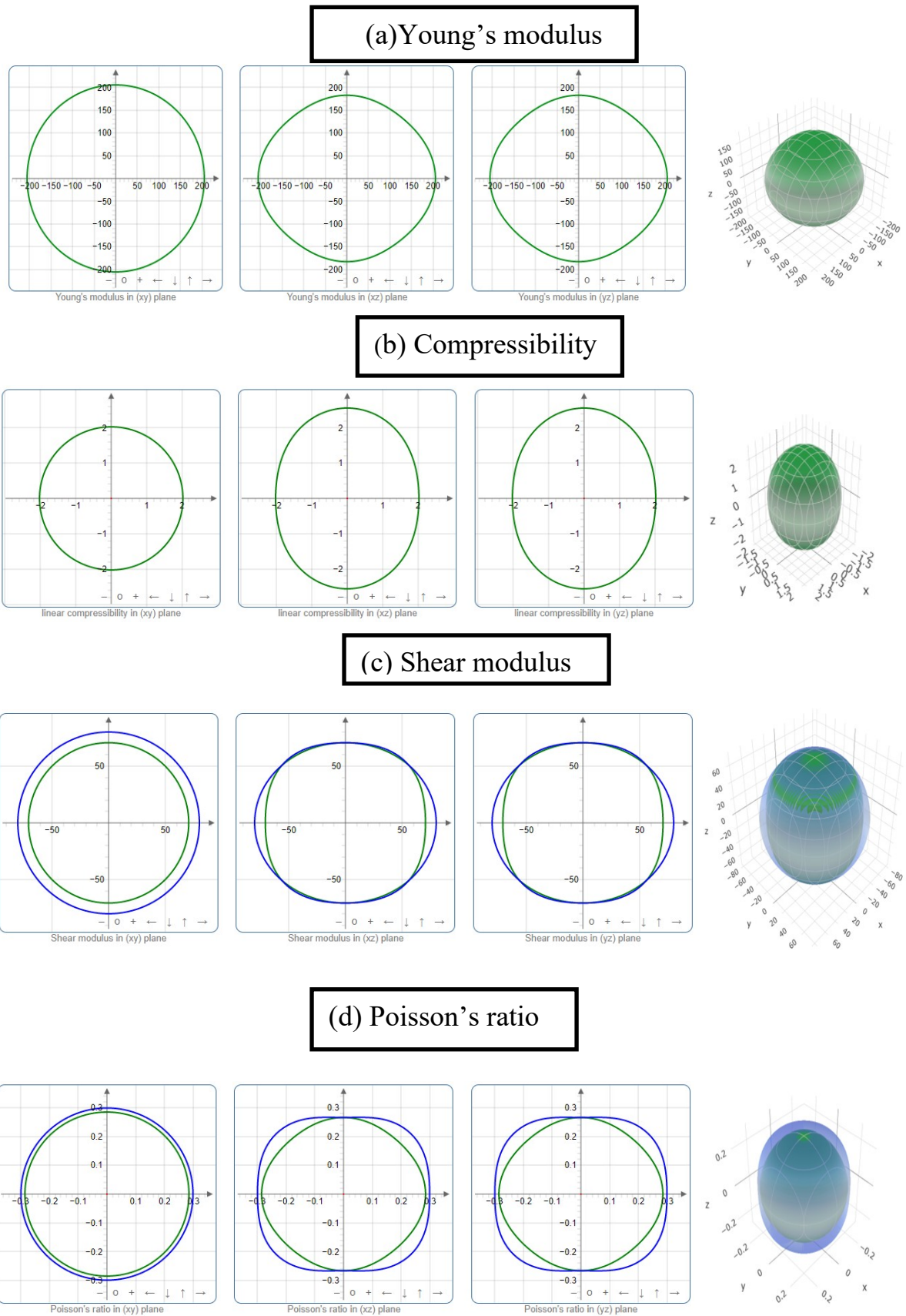
**(c) Shear modulus**



**(d) Poisson's ratio**

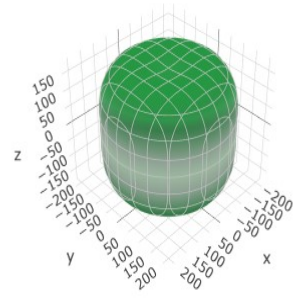
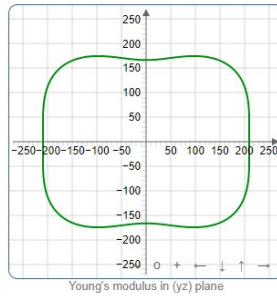
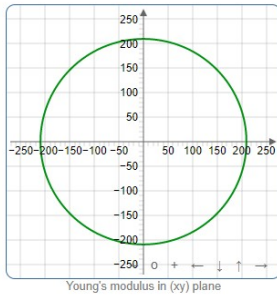


**Fig.S-5:** The 2D and 3D plots of (a)  $Y$ , (b)  $K$ , (c)  $G$  and (d)  $\nu$  of  $\text{Nb}_2\text{GeC}$  calculated using GGA PBEsol.

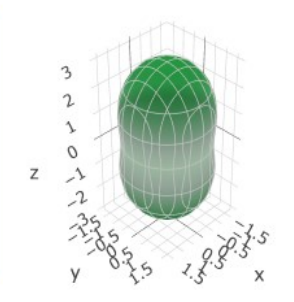
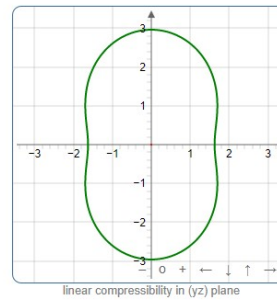
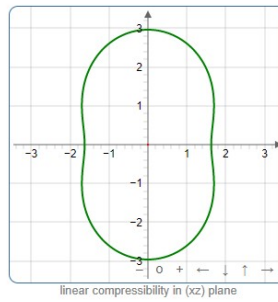
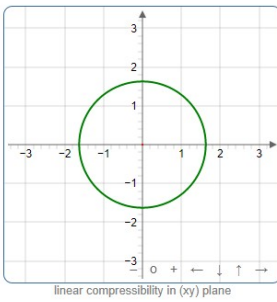


**Fig.S-6:** The 2D and 3D plots of (a)  $Y$ , (b)  $K$ , (c)  $G$  and (d)  $\nu$  of Nb<sub>2</sub>TiC calculated using GGA PBEsol.

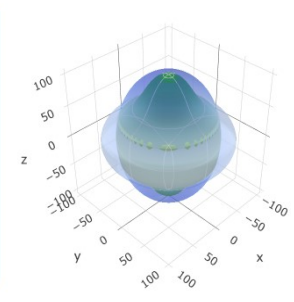
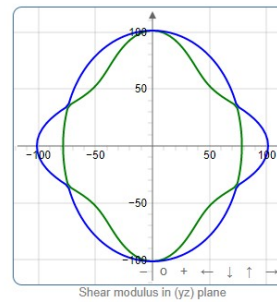
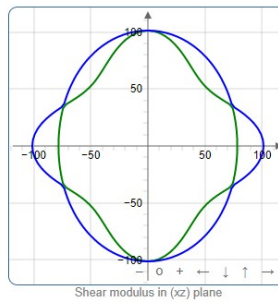
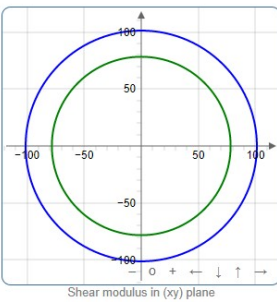
(a) Young's modulus



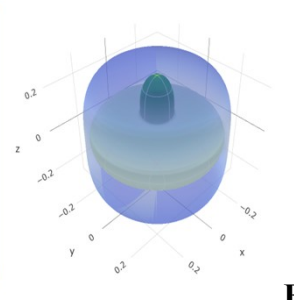
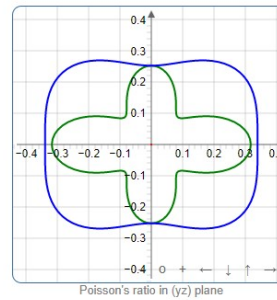
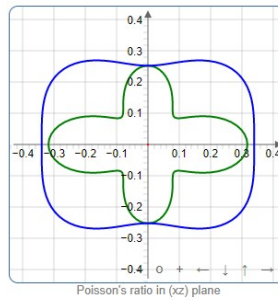
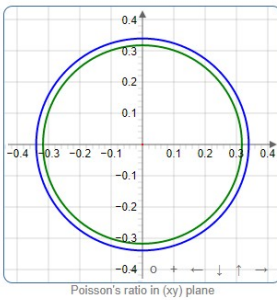
(b) Compressibility



(c) Shear modulus



(d) Poisson's ratio

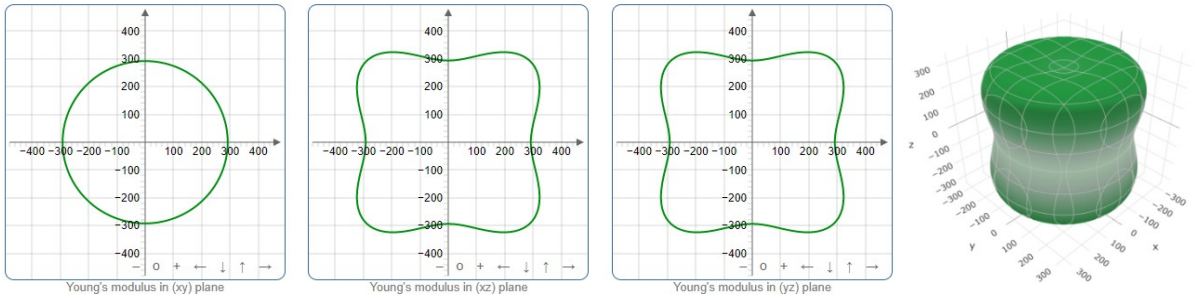


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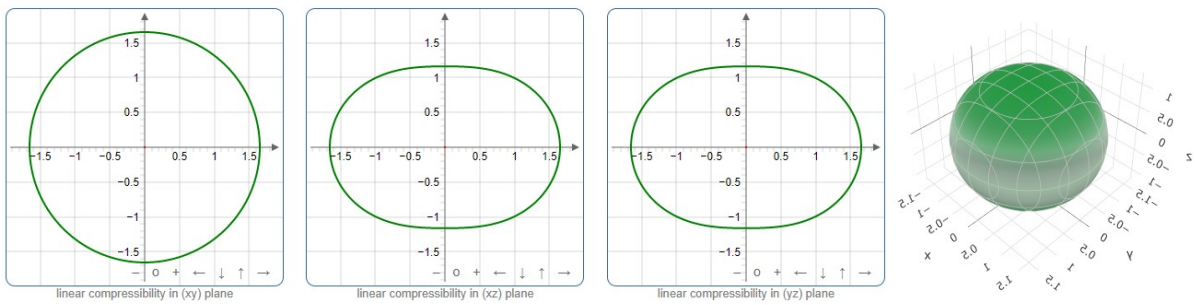
ig.S-7: The 2D and 3D plots of (a)  $Y$ , (b)  $K$ , (c)  $G$  and (d)  $\nu$  of  $Nb_2ZnC$  calculated using GGA PBEsol.



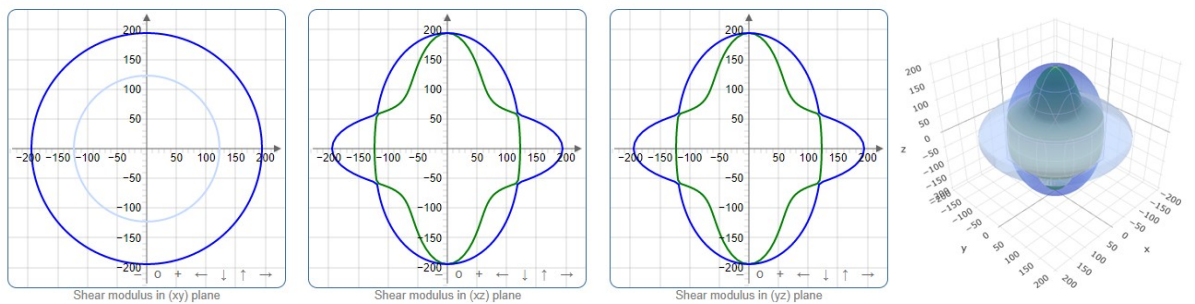
### (a) Young's modulus



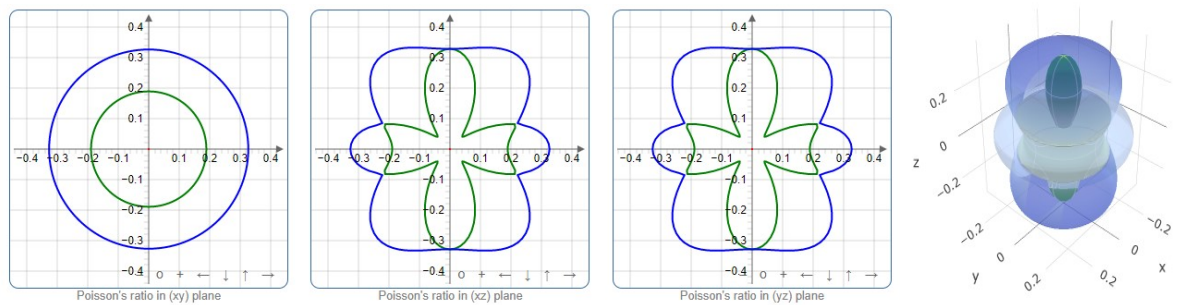
### (b) Compressibility



### (c) Shear modulus

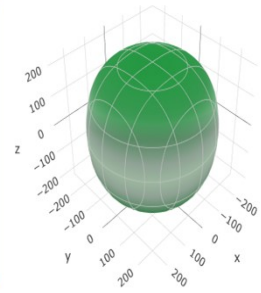
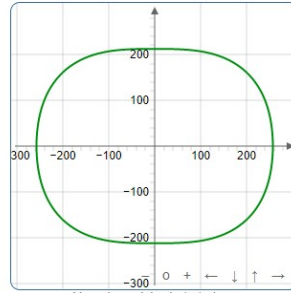
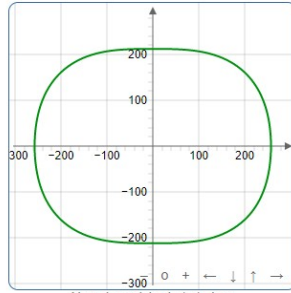
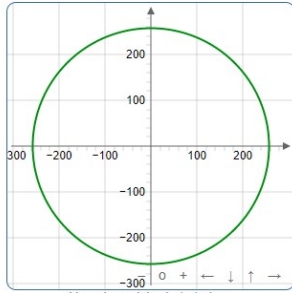


### (d) Poisson's ratio

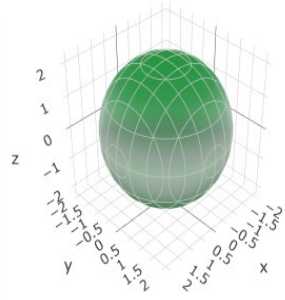
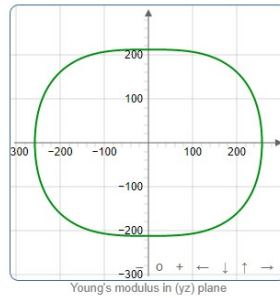
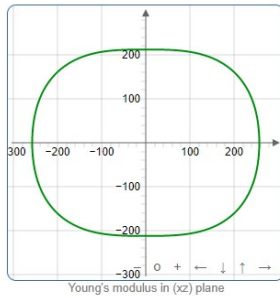
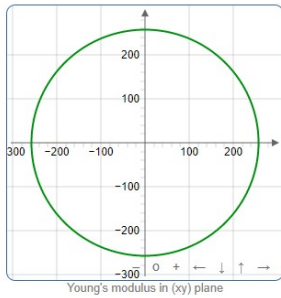


**Fig.S-8:** The 2D and 3D plots of (a)  $Y$ , (b)  $K$ , (c)  $G$  and (d)  $\nu$  of Nb<sub>2</sub>PC calculated using GGA PBEsol.

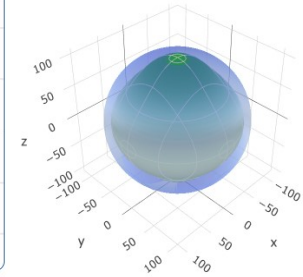
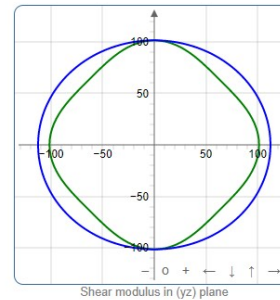
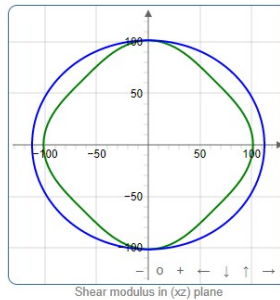
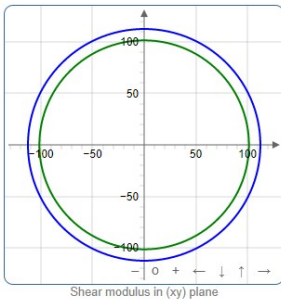
### (a) Young's modulus



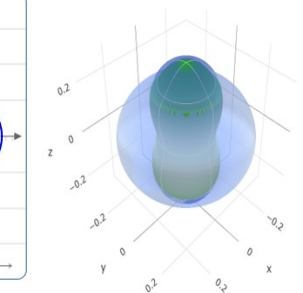
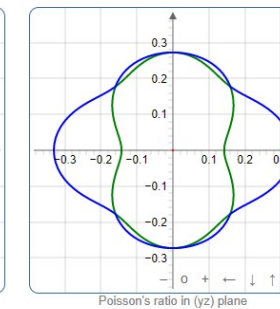
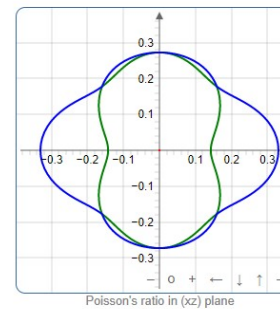
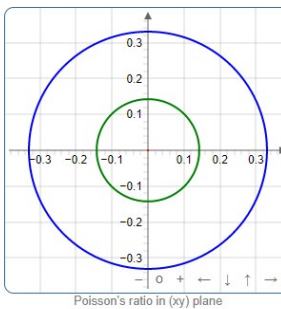
### (b) Compressibility



### (c) Shear modulus

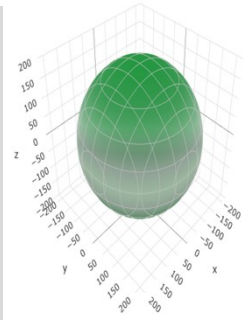
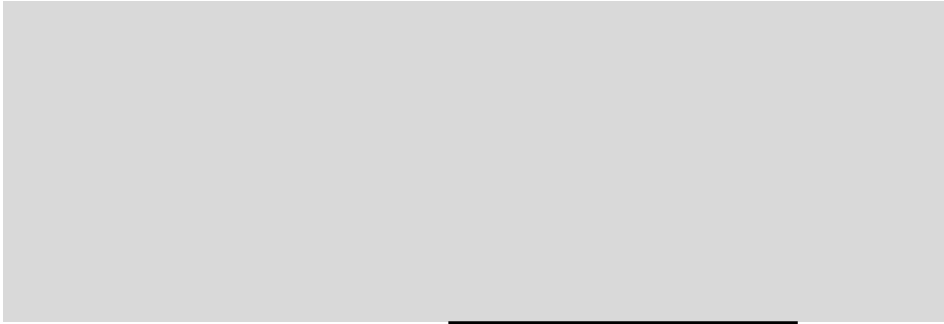


### (d) Poisson's ratio

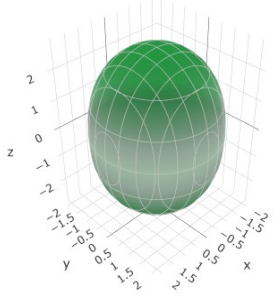
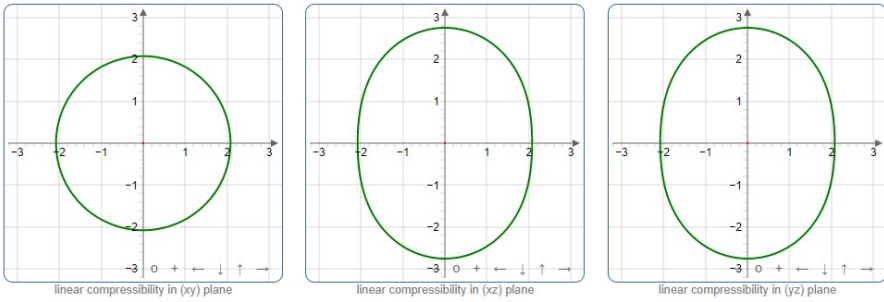


**Fig.S-9:** The 2D and 3D plots of (a) Y, (b) K, (c) G and (d)  $\nu$  of Nb<sub>2</sub>InC calculated using GGA PBEsol.

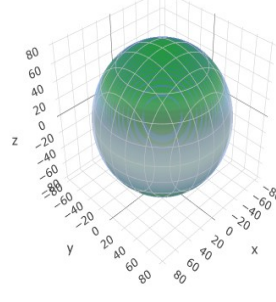
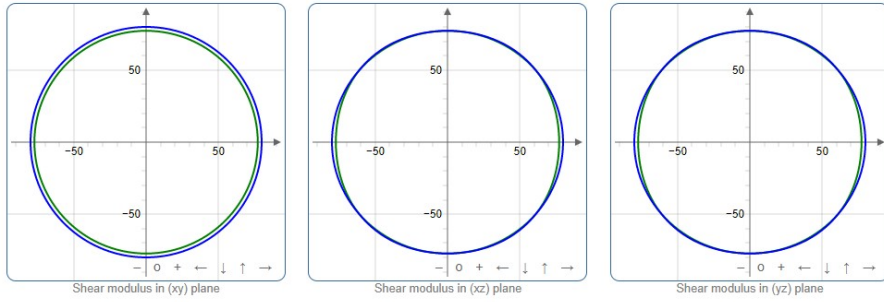
**(a) Young's modulus**



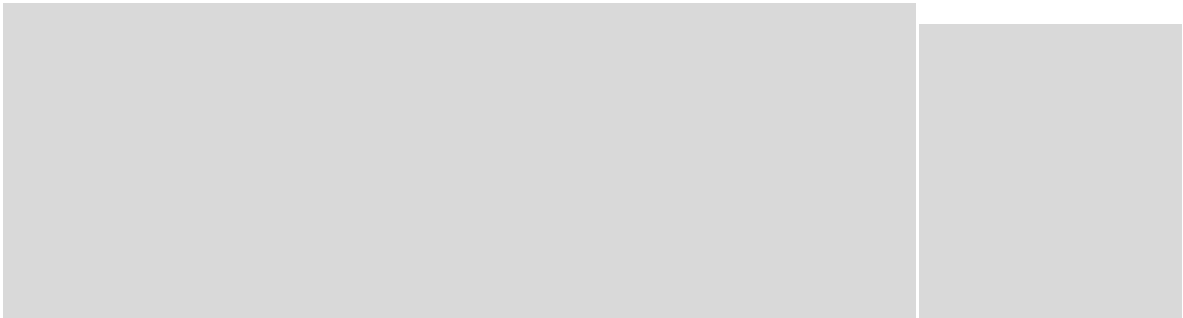
**(b) Compressibility**



**(c) Shear modulus**



**(d) Poisson's ratio**



**Fig.S-10:** The 2D and 3D plots of (a) Y, (b) K, (c) G and (d)  $\nu$  of Nb<sub>2</sub>CdC calculated using GGA PBEsol.

**Table S-1:** Mulliken atomic and bond overlap population (BOP) calculated using GGA-PBE.

Phases	Atoms	<i>s</i>	<i>p</i>	<i>d</i>	Total	Charge(e)	Bond	Bond number <i>n<sup>u</sup></i>	Bond overlap population <i>P<sup>u</sup></i>	Ref.
Nb <sub>2</sub> GaC	C	1.44	3.23	0.00	4.67	-0.67	C-Nb	4	0.93	This
	Ga	0.87	1.84	9.99	12.70	0.30				
	Nb	2.27	6.63	3.92	12.82	0.18				
Nb <sub>2</sub> GeC	C	1.44	3.22	0.00	4.66	-0.66	C-Nb	4	0.99	This
	Ge	1.01	2.54	10.00	13.55	0.45				
	Nb	2.33	6.61	3.96	12.89	0.11				
Nb <sub>2</sub> TlC	C	1.45	3.24	0.00	4.69	-0.69	C-Nb	4	0.94	This
	Tl	1.04	1.79	10.02	12.85	0.15				
	Nb	2.25	6.55	3.93	12.73	0.27				
Nb <sub>2</sub> ZnC	C	1.44	3.23	0.00	4.67	-0.67	C-Nb	4	0.92	This
	Zn	0.53	1.32	9.93	11.78	0.22				
	Nb	2.28	6.64	3.85	12.77	0.23				
Nb <sub>2</sub> PC	C	1.45	3.21	0.00	4.66	-0.66	C-Nb	4	1.01	This
	P	1.58	3.48	0.00	5.06	-0.06	P-Nb	4	0.98	
	Nb	2.24	6.45	3.95	12.64	0.36				
Nb <sub>2</sub> InC	C	1.44	3.22	0.00	4.66	-0.66	C-Nb	4	0.96	This
	In	0.98	1.81	9.97	12.77	0.23				
	Nb	2.23	6.64	3.92	12.79	0.21				
Nb <sub>2</sub> CdC	C	1.45	3.24	0.00	4.70	-0.70	C-Nb	4	0.99	This
	Cd	0.56	1.27	9.92	11.75	0.25				
	Nb	2.28	6.63	3.87	12.78	0.22				
Nb <sub>2</sub> AlC	C	1.43	3.21	0.00	4.65	-0.65	C-Nb	4	0.98	This
	Al	0.96	1.81	0.00	2.77	0.23				
	Nb	2.20	6.62	3.97	12.79	0.21				

**Table S-2:** Anisotropy factors  $A_1, A_2, A_3, k_c/k_a, B_a, B_c$  percentage anisotropy factors  $A_G$  and  $A_B$  and universal anisotropic index  $A^u$  calculated using GGA-PBE.

Phase	$A_1$	$A_2$	$A_3$	$B_a$	$B_c$	$K_c/k_a$	$A_B$	$A_G$	$A^u$	Ref.
Nb <sub>2</sub> GaC	0.669	1.0236	0.685	453.71	1017.29	1.07	0.003	0.013	0.134	This
Nb <sub>2</sub> GeC	0.2347	2.4706	0.5798	440.74	1886.74	1.51	0.003	0.016	1.846	This
Nb <sub>2</sub> TlC	1.0516	0.8875	0.9333	513.49	982.77	1.27	0.002	0.002	0.024	This
Nb <sub>2</sub> ZnC	0.7244	1.2866	0.9321	455.93	713.39	1.82	0.014	0.013	0.160	This
Nb <sub>2</sub> PC	0.552	1.584	0.874	526.67	1773.29	0.70	0.002	0.032	0.328	This
Nb <sub>2</sub> InC	0.827	0.903	0.747	440.46	941.15	1.05	0.003	0.005	0.050	This
Nb <sub>2</sub> CdC	1.123	0.969	0.648	523.91	884.98	1.32	0.005	0.001	0.019	This
Nb <sub>2</sub> AlC	0.618	1.236	0.764	491.08	1029.15	1.09	0.003	0.016	0.165	This

**Table S-3:** Calculated density ( $\rho$ ), longitudinal, transverse and average sound velocities ( $v_l$ ,  $v_t$ , and  $v_m$ , respectively), Debye temperature ( $\Theta_D$ ), minimum thermal conductivity ( $K_{min}$ ) and Grüneisen parameter ( $\gamma$ ) of  $Nb_2AC$  ( $A = Ga, Ge, Tl, Zn, P, In, Cd, Al$ ) calculated using GGA-PBE..

Phases	$\rho$ (g/cm <sup>3</sup> )	$v_l$ (m/s)	$v_t$ (m/s)	$v_m$ (m/s)	$\Theta_D$ (K)	$K_{min}$ (W/mk)	$\gamma$	$T_m$ (K)	Ref.
Nb <sub>2</sub> GaC	7.59	6660	3959	4031	533	0.91	1.41	1799	This
Nb <sub>2</sub> GeC	7.76	6064	3129	3239	428	0.75	2.06	1479	This
Nb <sub>2</sub> TlC	10.18	4975	2714	2794	354	0.59	1.71	1502	This
Nb <sub>2</sub> ZnC	7.43	6098	3382	3480	457	0.79	1.66	1553	This
Nb <sub>2</sub> PC	8.28	7140	4227	4682	736	1.81	1.41	2058	This
Nb <sub>2</sub> InC	11.49	5074	2978	3301	492	1.15	1.45	1667	This
Nb <sub>2</sub> CdC	8.06	5584	3130	3484	411	0.76	1.60	1487	This
Nb <sub>2</sub> AlC	6.34	7520	4474	4953	612	0.83	1.37	1897	This