Topological relations between crystal structures: a route to predicting inorganic materials

Natalia A. Kabanova,[a] Ekaterina A. Grishina,[a] Vladislav T. Osipov,[a] Valeria E. Pavlova,[a] Maria A. Solodovnikova,[a] Artem A. Kabanov,[a] Vladislav A. Blatov[a*]

[a]*Samara Center for Theoretical Material Science (SCTMS), Samara State Technical University, Molodogvardeyskaya St. 244, 443100 Samara, Russia*
blatov@topospro.com

Supplementary Materials

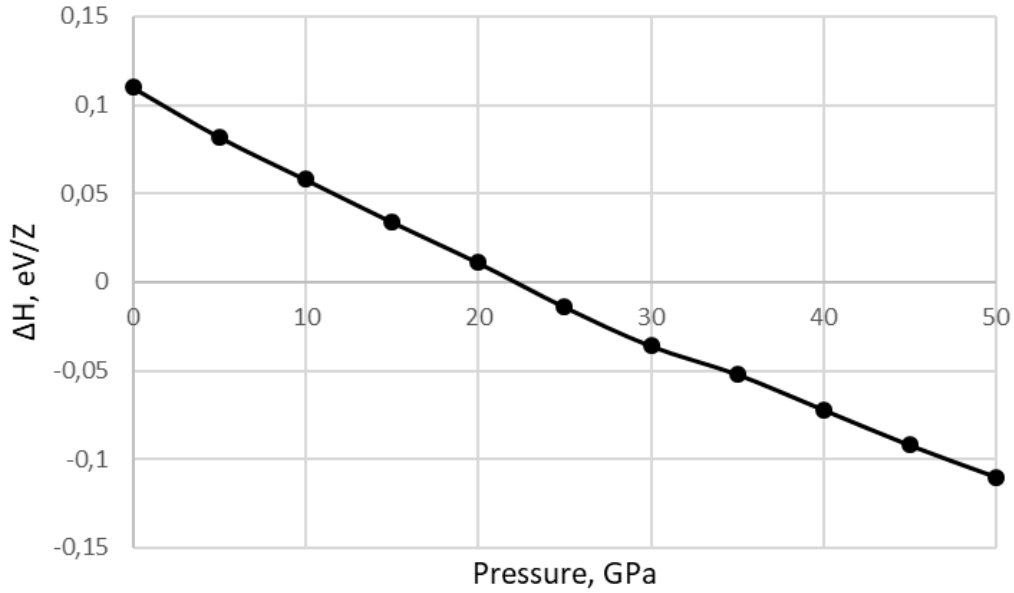

Figure S1. Dependence of lattice energy of RhB of the 7^2T3 topology on pressure.

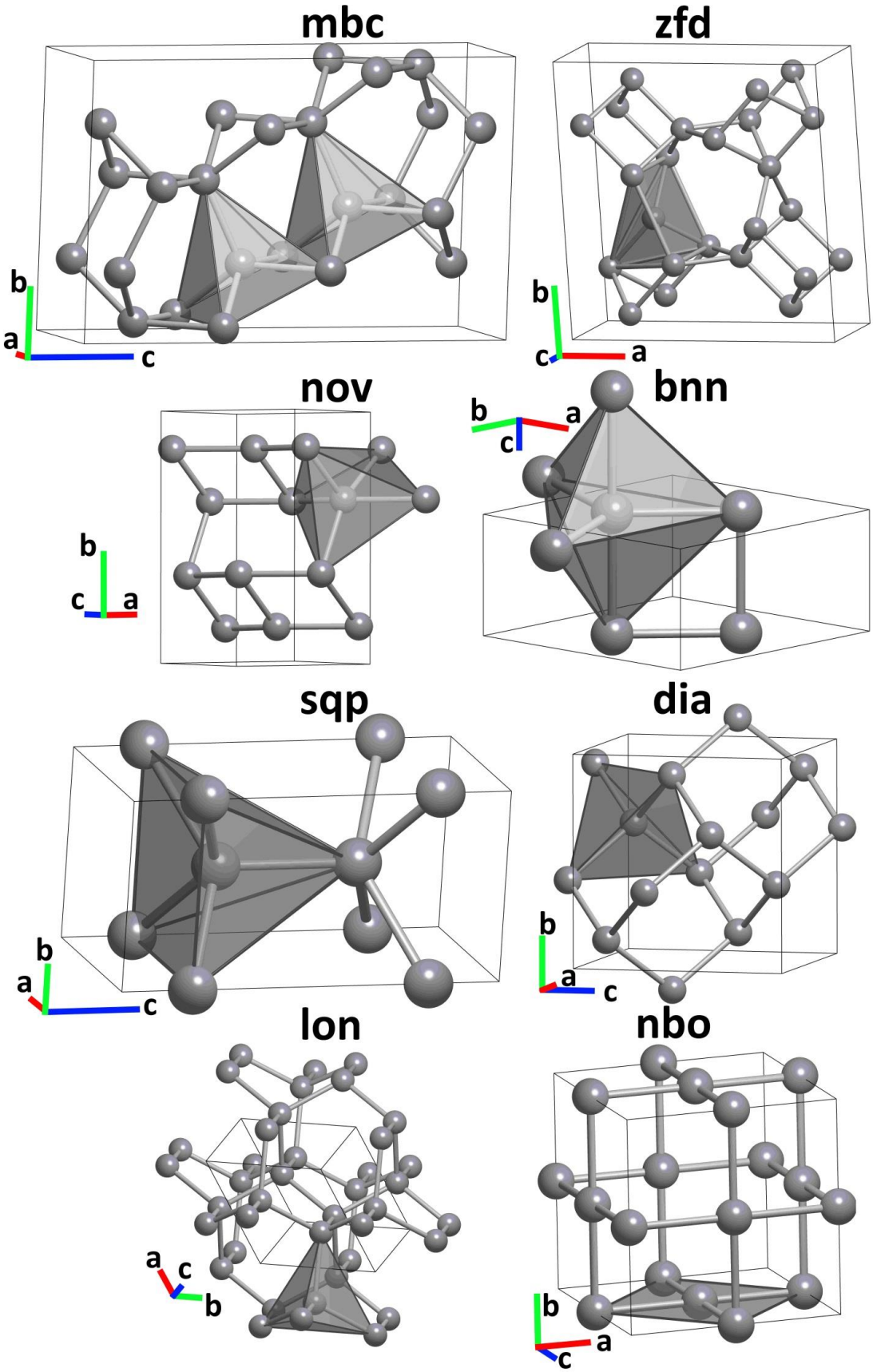

Figure S2. Topological types of some experimentally observed crystal structures of *MeX* (*Me* = Re, Ti or Rh; *X* = B, C, N or Si). The coordination polyhedra of inequivalent nodes are shaded in all nets.

Table S1. Mechanical properties of modeled *MeX* (*Me* = Re, Ti or Rh; *X* = B, C, N or Si) structures.

Topological type of net	Mechanical properties					
	B(GPa)	G(GPa)	E(GPa)	H1(GPa)	H2(GPa)	ν
ReB						
acs	358.8	231.80	572.17	26.3	26.0	0.2342
ste (anti-TiP)	330.6	149.35	389.42	20.5	11.8	0.3037
7^2T3	358.6	163.45	425.68	22.3	12.7	0.3022
TiB						
ste (TiP)	174.1	101.80	255.58	12.0	13.0	0.2553
pcu	142.8	88.90	220.87	10.2	12.9	0.2422
7^2T3	200.4	189.80	432.77	32.9	37.4	0.1401
RhB						
acs	274.50	58.10	162.82	9.3	0.5	0.4012
nia (anti-NiAs)	270.7	106.00	281.29	15.4	7.2	0.3268
pcu	253.6	39.35	112.24	6.4	-1.1	0.4262
ste (TiP)	255.8	103.50	273.59	14.8	7.5	0.3217
ste (anti-TiP)	257.6	39.45	112.60	6.5	-1.1	0.4272
7^2T3	239.1	88.80	237.06	13.1	5.7	0.3348
ReC						
acs	419.0	240.8	606.1	28.6	22.9	0.2589
nia (NiAs)	405.9	252.9	628.1	28.9	26.3	0.2421
nia (anti-NiAs)	398.6	129.8	351.2	19.7	6.3	0.3532
ste (TiP)	388.0	197.3	506.1	25.4	17.0	0.2826
ste (anti-TiP)	367.5	162.5	424.9	22.5	12.1	0.3073
TiC						
pcu	251	180.4	436.6	21.7	25.4	0.2101
ste (anti-TiP)	240.1	168.5	409.67	19.8	23.5	0.2156
nia (anti-NiAs)	239.4	155.1	382.65	17.6	20	0.2336
ste (TiP)	236.8	150.95	373.49	17.2	19.2	0.2371
nia (NiAs)	222.2	133.75	334.2	15.5	16.4	0.2493
dia	153.8	38.3	106.09	6.1	0.3	0.385
RhC						
dia	226.4	65.2	178.47	10.1	2.4	0.3686
acs	303.2	96.55	261.86	14.7	4.6	0.3561
nia (anti-NiAs)	234.2	63.1	173.7	9.9	1.9	0.3764
ReN						
nia (NiAs)	110.40	40.35	107.90	6.00	2.40	0.3371
ste (TiP)	394.90	214.30	544.41	26.40	19.60	0.2702
TiN						
nia (anti-NiAs)	275.50	161.00	404.26	19.00	17.80	0.2555
nia (NiAs)	298.00	144.05	372.18	19.10	12.60	0.2918
acs	274.00	148.65	377.67	18.40	15.20	0.2703
ste (TiP)	291.80	181.65	451.29	20.80	21.10	0.2422
ste (anti-TiP)	287.30	178.60	443.83	20.40	20.80	0.2425

pcu	302.10	182.40	455.54	21.10	20.30	0.2487
7^2T3	302.80	186.30	463.78	21.40	21.10	0.2447
RhN						
nia (anti-NiAs)	275.80	89.00	241.06	13.50	4.40	0.3543
nia (NiAs)	154.90	47.95	130.40	7.30	1.90	0.3597
acs	217.70	3.85	11.48	0.70	-3.00	0.4912
ste (anti-TiP)	261.50	30.25	87.38	5.00	-1.80	0.4443
ReSi						
svn	250.48	91.667	245.1	13.5	5.7	0.3369
TiSi						
pcu	112.1	28	77.54	4.4	-0.2	0.3847
ste (TiP)	101.3	41.45	109.43	5.9	3.2	0.3200
ste (anti-TiP)	116.7	62	158.02	7.8	7.7	0.2743
RhSi						
nia (NiAs)	181.9	65.65	175.81	9.7	4.0	0.339
ste (TiP)	186.6	30.95	87.99	5.1	-1.2	0.4214
7^2T3	175.1	35.45	99.63	5.7	-0.5	0.4052

B – bulk modulus, G – shear modulus, E – Young's modulus, ν – Poisson's ratio, H1 – Majnik-Oganov's hardness, H2 – Chen's hardness. The data for the most stable and experimentally obtained phases are shaded.