

Supporting Information

Structure prediction of aluminum nitride combining data mining and quantum mechanics

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Supplementary Tables

Table S1. Summary of the *AB* prototypes found in the ICSD

	Structure type	Reference	ICSD collection code		Structure type	Referenc e number	ICSD collection code
1.	AgCl	1	56541	46.	Li2O2	46	25530
2.	AlCe	2	57551	47.	LiAs	47	26472
3.	AlCu	3	40332	48.	LiSn	48	104782
4.	AlDy	4	57734	49.	Litharge (PbO)	49	53927
5.	AlLi	5	240114	50.	Massicot (PbO)	50	15402
6.	AlTh	6	58179	51.	MnP	51	30412
7.	AuCd	7	58409	52.	MoB	52	24280
8.	BeO`	8	18147	53.	MoC	53	44987
9.	BiI	9	1558	54.	Na2O2	54	25526
10.	BiIn	10	58790	55.	NaHS	55	26732
11.	BiSe	11	20458	56.	NaP	56	14009
12.	BN	12	35538	57.	NaPb	57	105156
13.	CO	13	26962	58.	NaTl	58	105169
14.	CoAs	14	15065	59.	NbAs	59	16585
15.	CoGe	15	43677	60.	NbO	60	14338
16.	CoO	16	53059	61.	NiAs	61	31062
17.	CoSn	17	102671	62.	NiO	62	92127
18.	CrSe	18	24792	63.	NiS	63	29312
19.	CuCl	19	78271	64.	NiTi	64	105414
20.	CuO	20	31059	65.	NS	65	4025
21.	CuSe	21	240	66.	P4S4	66	1703
22.	CuTe	22	42591	67.	PdO	67	26598
23.	CuTi	23	103128	68.	PtTe	68	41370
24.	FeB	24	30449	69.	Rb2C2	69	51529
25.	FeS2H	25	68847	70.	SiC4H	70	24170
26.	FeSi	26	36188	71.	SiC6H	71	15325
27.	FeSmP24	27	87500	72.	SrSi	72	25534
28.	GaS	28	59	73.	ThTl	73	106158
29.	GeAs	29	17033	74.	Tl2Se2	74	30219
30.	GeK	30	43515	75.	TiAs	75	16773
31.	GeS	31	38165	76.	TlI	76	26761
32.	GeTeSubcell	32	43202	77.	TlTe	77	69027
33.	GeTeSupercell	33	56042	78.	ZnAs	78	431
34.	HgCl	34	36195	79.	ZnS2H	61	31061
35.	HgK	35	104302	80.	ZnS15R	79	37375
36.	HgNa	36	104326	81.	ZnS21R	79	37376
37.	HgO	37	40316	82.	ZnS(cF8)	80	53943
38.	HgS	38	31129	83.	ZrCl	81	20145

39.	IrTa	39	104565	84.	ZrSb	82	52404
40.	IrU	40	104584	85.	CsCl	83	53847
41.	KCN	41	38443	86.	GeP	84	17032
42.	KOH	42	61047	87.	WC	85	22258
43.	LaI	43	83678	88.	NaCl	86	1913
44.	LaS	44	69581	89.	5-5		
45.	LaSi	45	408030				

Supplementary Figures

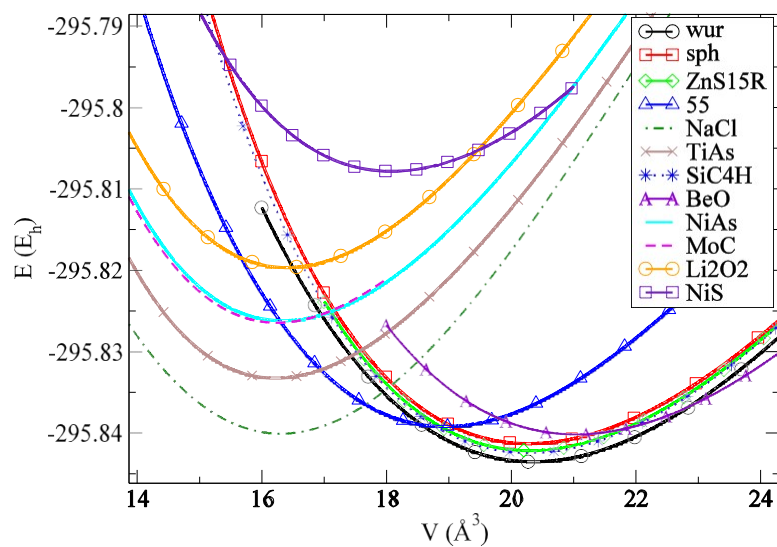


Fig. S1. Calculated $E(V)$ curves for the optimized AlN structure types obtained using LDA functional. Energies per formula unit are given in hartrees (E_h).

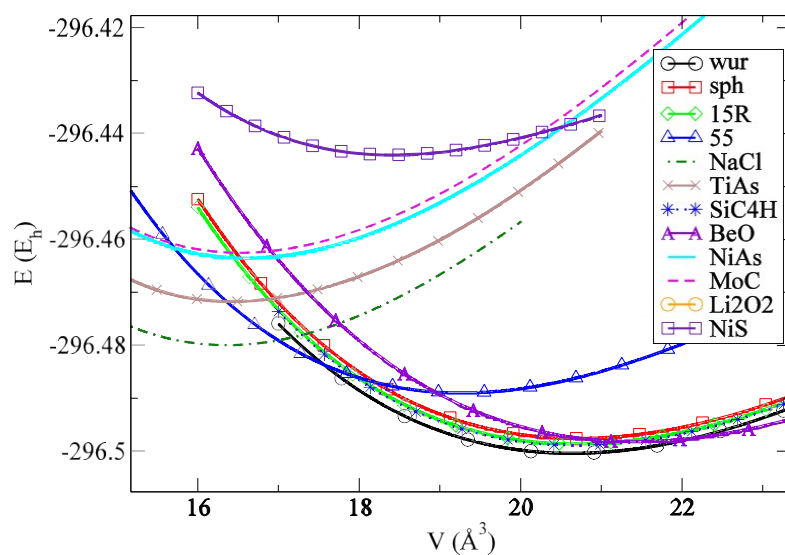


Fig. S2. Calculated $E(V)$ curves for the optimized AlN structure types obtained using HF functional. Energies per formula unit are given in hartrees (E_h),

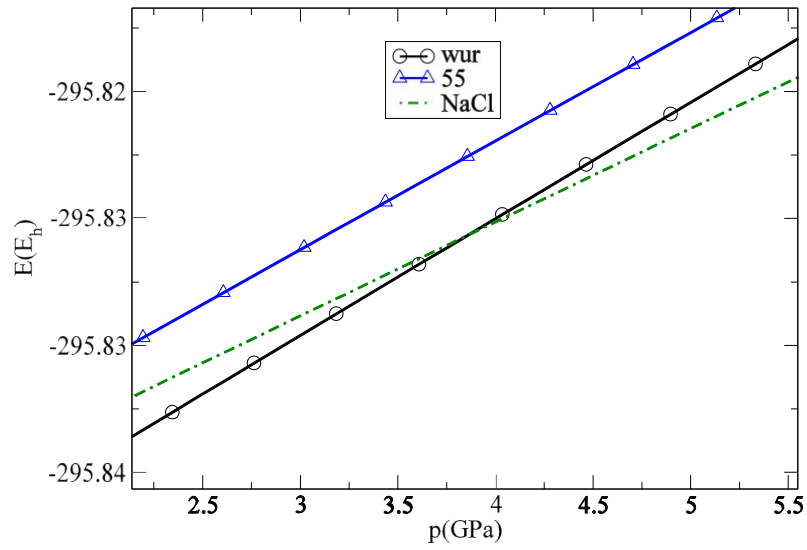


Fig. S3. $H(p)$ curves at LDA level for the most relevant structure types at high pressures. Energies per formula unit are given in hartrees (Eh).

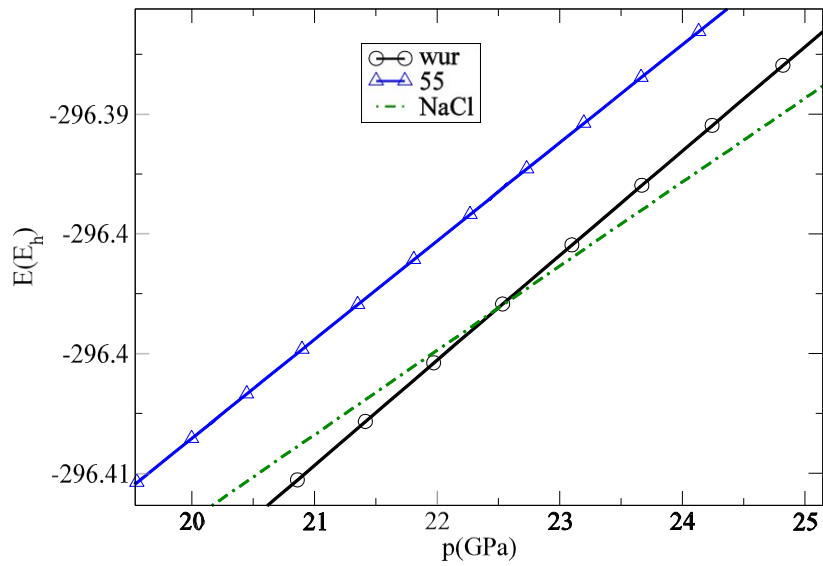


Fig. S4. $H(p)$ curves at HF level for the most relevant structure types at high pressures. Energies per formula unit are given in hartrees (Eh).

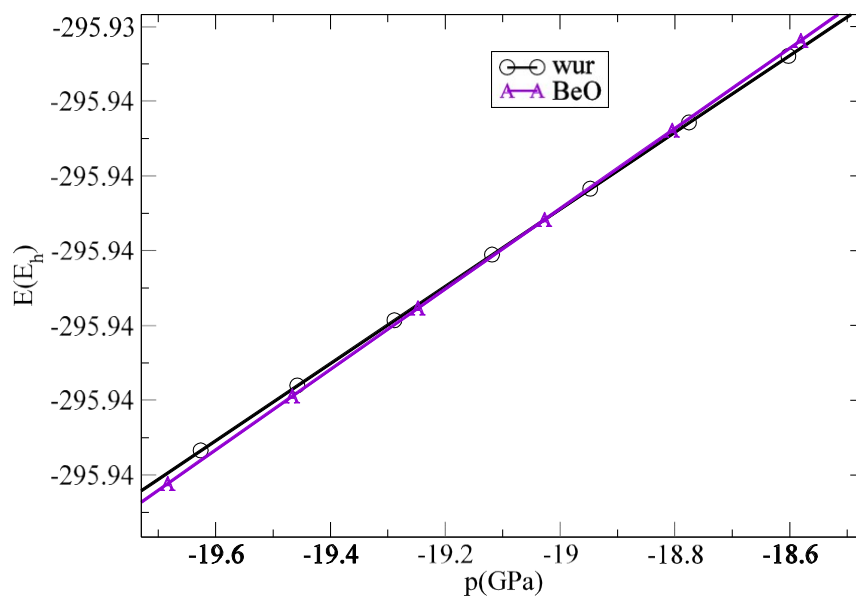


Fig. S5. $H(p)$ curves at LDA level for the most relevant structure types at the negative pressure. Energies per formula unit are given in hartrees (Eh).

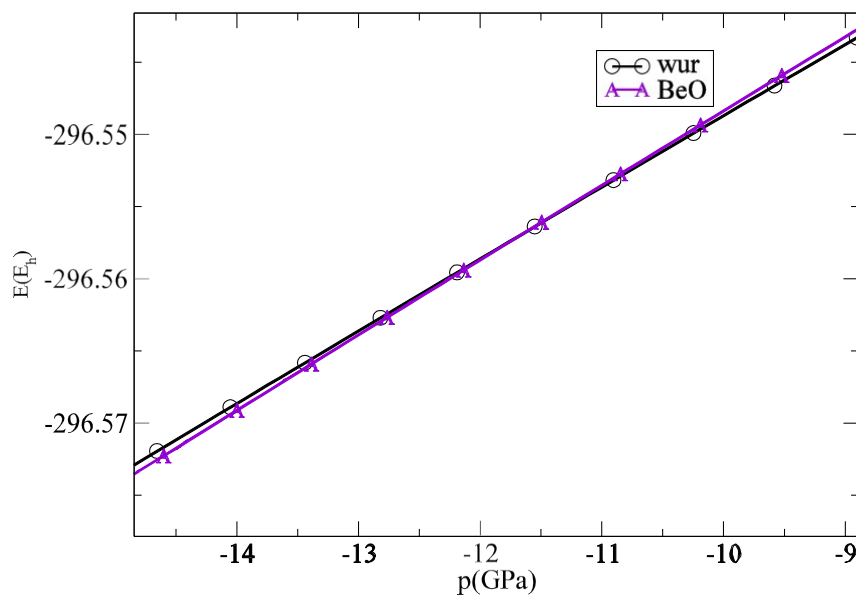


Fig. S6. $H(p)$ curves at HF level for the most relevant structure types at the negative pressure. Energies per formula unit are given in hartrees (Eh).

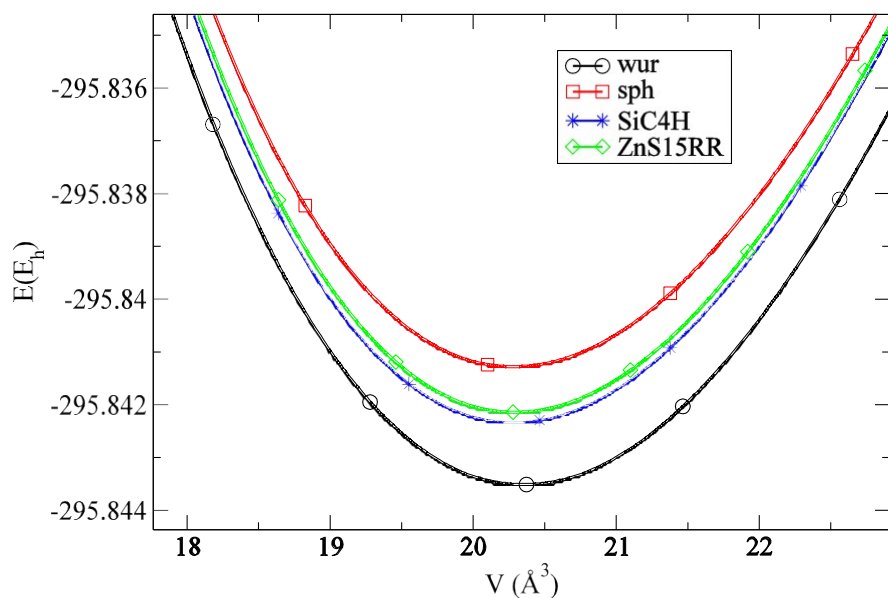


Fig. S7. Calculated $E(V)$ curves for the experimentally observed AlN structures and predicted AlN polytypes 4H and 15R obtained using LDA functional. Energies per formula unit are given in hartrees (E_h).

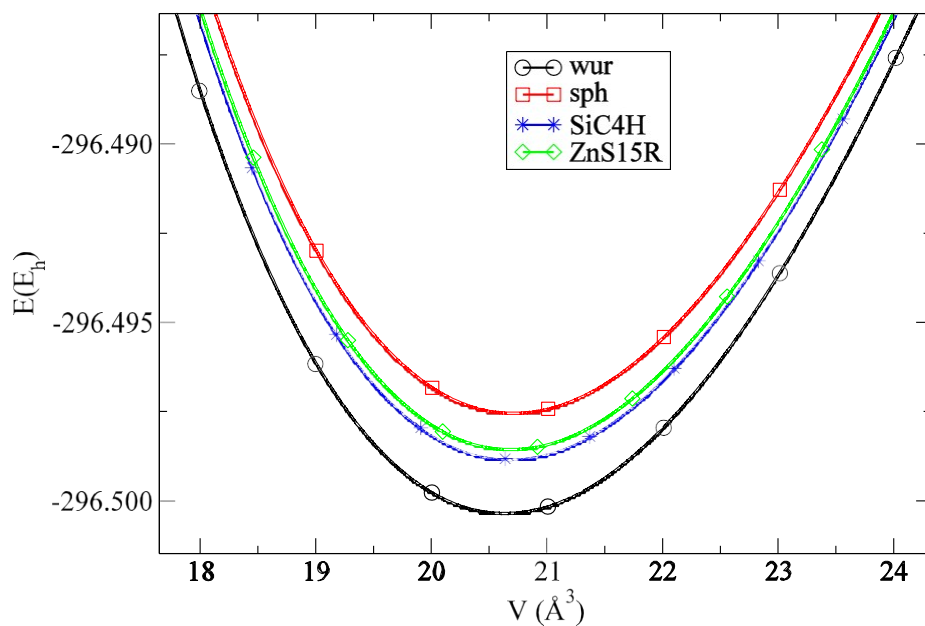


Fig. S8. Calculated $E(V)$ curves for the experimentally observed AlN structures and predicted AlN polytypes 4H and 15R obtained using HF functional. Energies per formula unit are given in hartrees (E_h).

Supplementary References

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