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Pressure-induced novel semiconductor materials with high dielectric constant in ZrN_4: a first-principles study

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Table S1 The lattice parameters and Wyckoff positions of the eight novel phases(Å).

Phase	Lattice parameters (Å, degree)	Wyckoff positions				
		atom	site	x	y	z
α-$P1$	a = 6.433, b =3.586, c =8.961	Zr1	1a	0.211	0.601	0.608
	α = 88.9°, β = 103.7°, γ = 90.6°	Zr2	1a	0.815	0.098	0.511
		N1	1a	0.052	0.142	0.085
		N2	1a	0.643	0.682	0.009
		N3	1a	0.506	0.484	-0.003
		N4	1a	0.195	0.989	0.151
		N5	1a	0.934	0.618	0.442
		N6	1a	0.469	0.242	0.520
		N7	1a	0.095	0.108	0.678
		N8	1a	0.527	0.959	0.603
P_4/mmm	a =3.711, b =3.676, c =4.020	Zr1	1b	1.000	1.000	0.500
	α =90.0°, β =90.0°, γ =90.0°	N1	4i	1.000	0.500	0.152
α-$P\bar{1}$	a =3.998, b =4.909, c =5.161	Zr1	2i	-0.733	1.166	-1.282
	α =76.2°, β =90.1°, γ =97.8°	N1	2i	-0.297	0.602	-1.249
		N2	2i	-0.239	1.107	-1.414
		N3	2i	0.040	1.531	-1.885
		N4	2i	-0.304	0.877	-1.175
α-$P2_1/m$	a =4.381, b =4.930, c =4.017	Zr1	2e	0.780	0.250	1.417
	α =90.0°, β =91.8°, γ =90.0°	N1	2e	0.699	0.750	0.988
		N2	2e	0.317	0.250	1.658
		N3	4f	0.858	0.511	1.892
β-$P\bar{1}$	a =4.976, b =4.459, c =4.797	Zr1	2i	0.279	0.713	0.783
	α =77.8°, β =100.8°, γ =111.4°	N1	2i	-0.032	-0.058	0.879
		N2	2i	-0.237	0.032	0.687
		N3	2i	-0.244	0.345	0.720
		N4	2i	0.524	0.715	1.193
γ-$P\bar{1}$	a =4.111, b =4.962, c =4.443	Zr1	2i	0.291	0.833	0.788
	α =78.6°, β =97.0°, γ =87.9°	N1	2i	0.241	0.375	0.401
		N2	2i	0.757	0.635	0.267
		N3	2i	0.902	0.359	0.777
		N4	2i	0.205	0.905	0.281
β-$P2_1/m$	a =4.730, b =4.898, c =4.118	Zr1	2e	1.218	0.250	1.505
	α =90.0°, β =109.2°, γ =90.0°	N1	2e	1.288	0.750	1.119
		N2	2e	1.696	0.250	1.529
		N3	4f	0.858	0.490	0.046
β-$P1$	a =4.970, b =4.462, c =7.041	Zr1	1a	0.728	0.933	0.315
	α =83.6°, β =74.5°, γ =107.4°	Zr2	la	0.082	0.347	0.708
		Zr3	la	0.446	0.869	0.960
		N1	la	0.436	0.355	0.067
		N2	la	0.718	0.308	0.044

N3	la	0.261	0.920	0.322
N4	la	0.111	0.813	0.540
N5	la	0.651	0.361	0.439
N6	la	0.594	0.345	0.663
N7	la	0.404	0.435	0.399
N8	la	0.578	0.651	0.691
N9	la	0.268	0.248	0.274
N10	la	0.863	0.915	0.586
N11	la	0.972	0.601	0.965
N12	la	0.892	0.875	0.983

Table S2 Variation of lattice constants normalized with respect to their respective ground state values (i.e. $\Delta a=(a_{150}-a_0)/a_0\times100\%$, $\Delta b=(b_{150}-b_0)/b_0\times100\%$, $\Delta c=(c_{150}-c_0)/c_0\times100\%$) for ZrN_4 semiconductor phases at 150 GPa.

Phase	Δa	Δb	Δc
α-$P\bar{1}$	-22.23	-15.28	-2.92
β-$P\bar{1}$	-20.85	-18.25	5.93
γ-$P\bar{1}$	-10.72	-11.2	-8.08
β-$P1$	-14.79	-6.21	-15.81

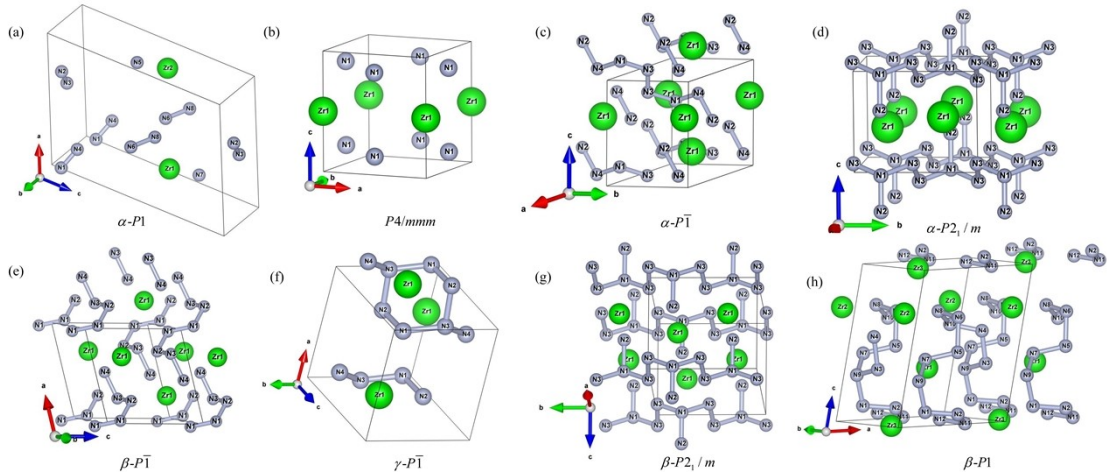

Fig. S1 Configurations of the nitrogen chains in (a) α-$P1$, (b) $P4/mmm$, (c) α-$P\bar{1}$, (d) α-$P2_1/m$, (e) β-$P\bar{1}$, (f) γ-$P\bar{1}$, (g) β-$P2_1/m$, and (h) β-$P1$ phase for ZrN_4 at 0 GPa. The green and gray balls denote the Zr and N atoms, respectively.

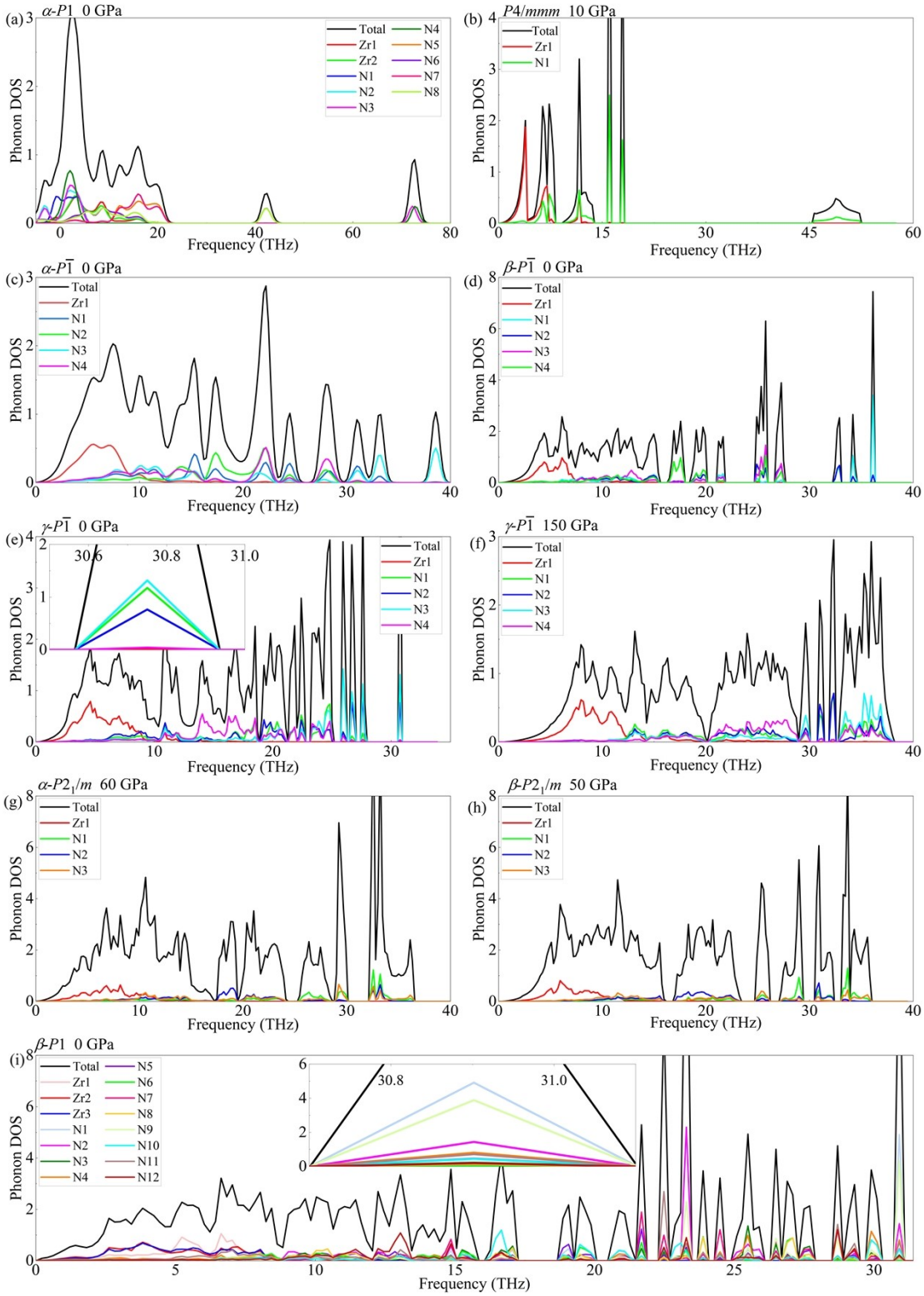

Fig. S2 Total phonon DOS and Partial phonon DOS for Zr and N atoms in ZrN_4. The inset in (e) and (i) shows the phonon DOS in the frequency range of 30.5–31 GPa and 30.7–31.1 GPa, respectively.

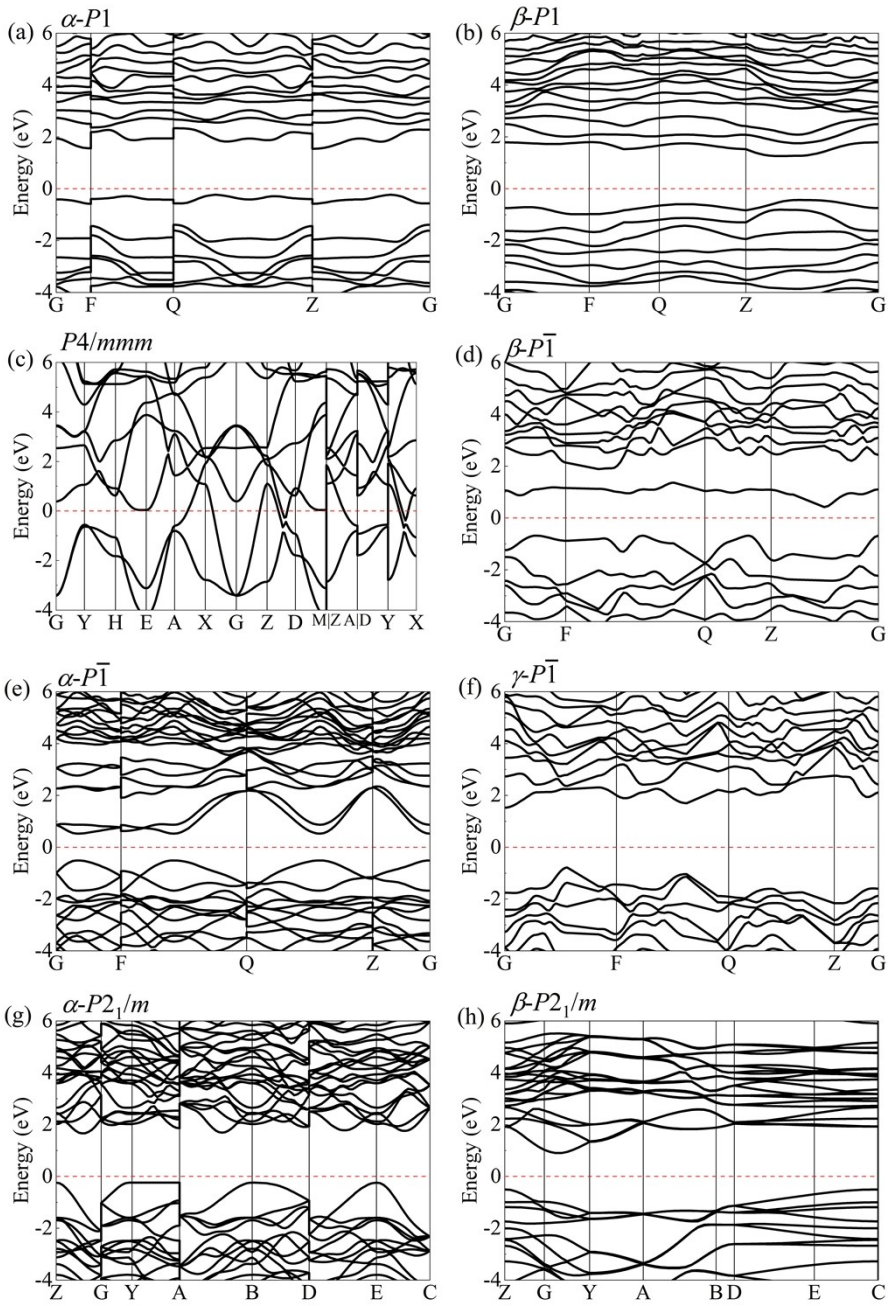

Fig. S3 The band of (a) α-$P1$, (b) β-$P1$, (c) $P4/mmm$, (d) β-$P\bar{1}$, (e) α-$P\bar{1}$, (f) γ-$P\bar{1}$, (g) α-$P2_1/m$, and (h) β-$P2_1/m$ under HSE06 functional.