

## Supporting Information

**Table S1.** Second-order elastic constants (GPa), piezoelectric components ( $\text{C m}^{-2}$ ) and dielectric components (dimensionless) of wurtzite-2H, calculated at different pressures (GPa) and related properties: bulk modulus (Voigt, Reuss and VRH, GPa), shear modulus (Voigt, Reuss and VRH, GPa), Young's moduli (VRH, GPa), Poisson's ratio, Pugh ratio  $k$ , Vickers hardness  $H_v$  (GPa) and wave velocities (primary and secondary,  $\text{km s}^{-1}$ ). Density values ( $\rho$ ,  $\text{kg m}^{-3}$ ) are also reported.

	Pressure (GPa)										
	22.05	17.15	12.49	8.49	5.05	1.77	0.43	-0.51	-2.75	-4.69	-6.37
$C_{11}$	176.22	165.85	154.72	144.02	134.05	123.56	119.10	115.64	107.20	99.20	91.35
$C_{12}$	137.54	119.81	102.32	87.05	73.30	61.34	55.81	52.02	42.48	34.71	27.87
$C_{13}$	126.66	107.96	90.65	75.65	62.38	49.29	44.35	40.81	32.83	26.26	20.77
$C_{33}$	212.92	196.69	181.05	168.05	155.16	142.83	136.67	132.32	121.34	110.75	100.57
$C_{44}$	17.04	20.33	23.10	25.17	26.71	27.73	28.09	28.26	28.57	28.48	28.45
$e_{33}$	0.719	0.664	0.589	0.508	0.416	0.303	0.246	0.202	0.076	-0.064	-0.221
$e_{31}$	-0.405	-0.375	-0.335	-0.289	-0.240	-0.184	-0.155	-0.131	-0.068	0.002	0.078
$e_{15}$	-0.353	-0.318	-0.280	-0.241	-0.196	-0.143	-0.117	-0.097	-0.042	0.016	0.086
$\epsilon_{11}$	4.264	4.253	4.243	4.234	4.235	4.241	4.245	4.250	4.263	4.281	4.303
$\epsilon_{33}$	4.349	4.318	4.299	4.280	4.273	4.271	4.273	4.275	4.283	4.296	4.312
$\rho$	4541	4393	4239	4091	3950	3801	3735	3686	3563	3445	3333
$K_V$	134.97	121.88	109.20	97.98	87.68	77.68	73.49	70.44	63.17	56.86	51.14
$\mu_V$	33.34	34.15	34.52	34.53	34.30	33.53	33.14	32.74	31.70	30.29	28.80
$K_R$	134.48	121.62	109.03	97.86	87.59	77.64	73.46	70.41	63.15	56.85	51.14
$\mu_R$	31.80	32.76	33.28	33.38	33.25	32.48	32.15	31.80	30.90	29.62	28.30
$K_{VRH}$	134.73	121.75	109.11	97.92	87.64	77.66	73.47	70.43	63.16	56.85	51.14
$\mu_{VRH}$	32.57	33.46	33.90	33.95	33.77	33.01	32.64	32.27	31.30	29.96	28.55
$E_{VRH}$	90.42	91.95	92.15	91.30	89.78	86.73	85.30	83.98	80.58	76.44	72.21
$U_{VRH}$	0.388	0.374	0.359	0.345	0.329	0.314	0.306	0.301	0.287	0.276	0.265
$k$	0.24	0.27	0.31	0.35	0.39	0.43	0.44	0.46	0.50	0.53	0.56
$H_v$	-0.09	0.44	1.00	1.55	2.14	2.68	2.95	3.12	3.59	3.91	4.18
$v_p$	2.678	2.760	2.828	2.881	2.924	2.947	2.956	2.959	2.964	2.949	2.927
$v_s$	6.836	6.676	6.505	6.341	6.175	5.994	5.913	5.851	5.694	5.541	5.387