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Supporting information for article:

Thermomechanical, electronic and thermodynamic properties of ZnS cubic polymorphs: an *ab initio* investigation on the zinc-blende–rock-salt phase transition

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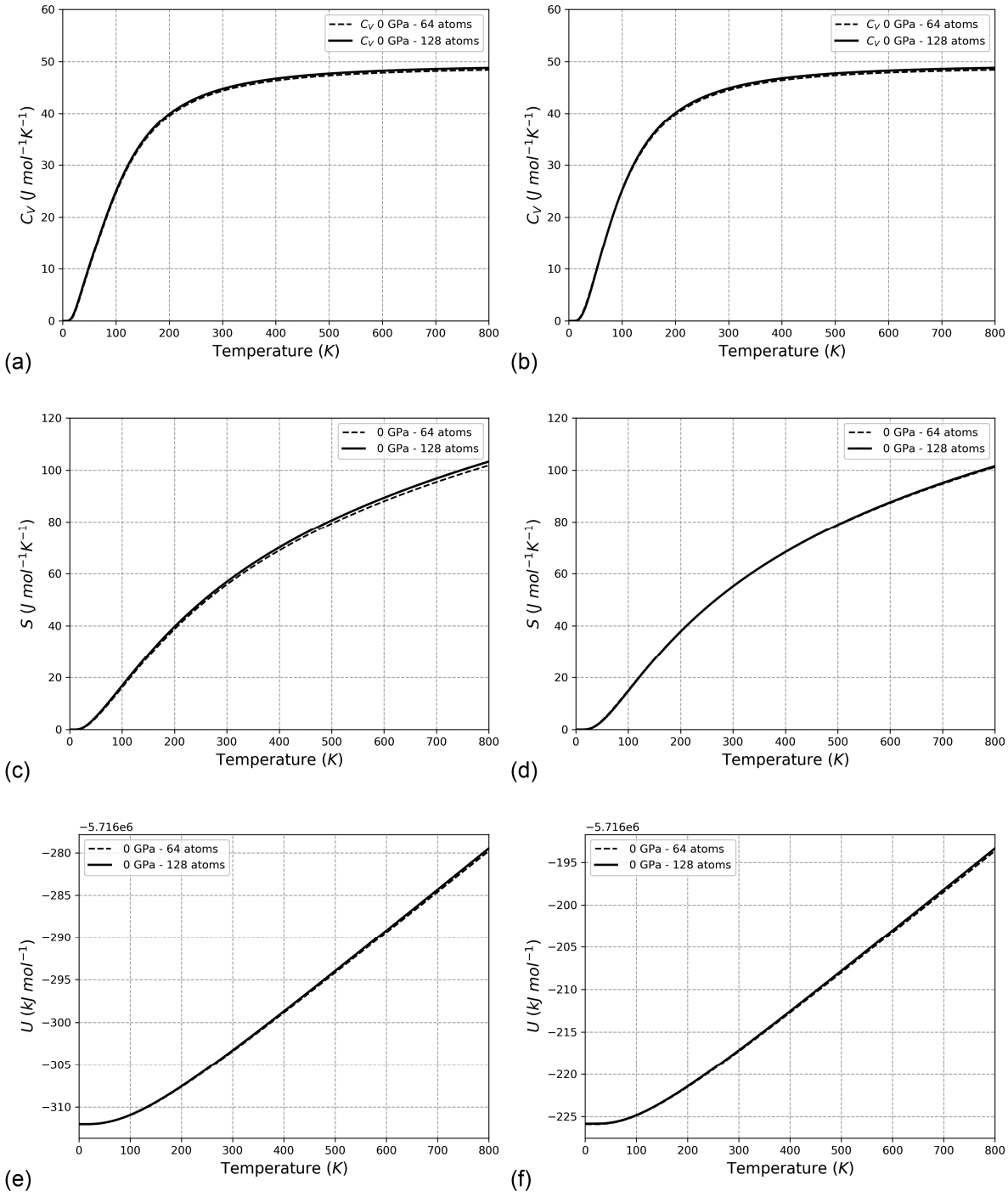

Figure S1 Harmonic approximation properties of sphalerite (a,c,e) and rock-salt ZnS (b,d,f), calculated employing two supercells with 64 and 128 atoms. (a,b) Isochoric heat capacity C_V, (c,d) entropy S and (e,f) internal energy U.

Table S1 Second-order elastic constants (GPa), piezoelectric components (C m^{-2}) and dielectric components (dimensionless) of sphalerite and rock-salt ZnS, 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 and wave velocities (primary and secondary, km s^{-1}). Density values (ρ, kg m^{-3}) are also reported.

						Sphalerite					
P	21.30	16.23	11.81	7.95	4.59	1.67	0.05	-0.87	-3.06	-4.95	-6.57
C_{11}	164.973	150.270	137.063	125.274	114.589	104.683	99.076	95.988	88.136	81.359	75.107
C_{12}	141.782	122.533	105.885	91.119	77.858	66.219	59.519	55.971	46.899	39.028	32.068
C_{44}	38.071	41.814	44.556	46.278	46.968	47.192	47.007	46.764	45.660	44.167	41.902
e_{14}	0.586	0.517	0.444	0.365	0.281	0.192	0.132	0.093	-0.16	-0.142	-0.278
ε_{11}	4.290	4.277	4.267	4.258	4.261	4.266	4.271	4.275	4.288	4.307	4.329
ρ	4539	4379	4225	4078	3939	3806	3722	3678	3557	3438	3328
K_V	149.51	131.78	116.28	102.50	90.10	79.04	72.70	69.31	60.64	53.14	46.41
μ_V	27.48	30.64	32.97	34.60	35.53	36.01	36.12	36.06	35.64	34.97	33.75
K_R	149.51	131.78	116.28	102.50	90.10	79.04	72.70	69.31	60.64	53.14	46.41
μ_R	19.90	23.15	25.56	27.48	28.94	29.84	30.31	30.47	30.73	30.79	30.39
K_{VRH}	149.51	131.78	116.28	102.50	90.10	79.04	72.70	69.31	60.64	53.14	46.41
μ_{VRH}	23.69	26.89	29.26	31.04	32.23	32.92	33.21	33.26	33.19	32.88	32.07
E_{VRH}	67.50	75.54	81.00	84.58	86.40	86.73	86.48	86.03	84.20	81.76	78.20
υ_{VRH}	0.425	0.404	0.384	0.362	0.340	0.317	0.302	0.293	0.269	0.244	0.219
v_p	2.285	2.478	2.632	2.759	2.860	2.941	2.987	3.007	3.055	3.093	3.104
v_s	12.141	11.781	11.440	11.107	10.772	10.441	10.242	10.125	9.807	9.514	9.203
						Rock-salt ZnS					
P	25.65	19.48	14.14	9.51	5.51	2.07	0.18	-0.90	-3.44	-5.61	-7.46
C_{11}	336.351	287.054	245.385	208.789	176.729	149.165	132.692	124.013	102.500	83.722	66.812
C_{12}	105.308	93.712	85.122	77.397	70.475	63.441	60.188	58.200	53.176	49.165	45.297
C_{44}	69.458	67.360	65.837	63.795	62.296	60.693	59.750	59.172	57.683	55.986	54.280
e_{14}	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
ε_{11}	6.446	6.446	6.443	6.470	6.508	6.563	6.606	6.632	6.727	6.812	6.931
ρ	5483	5288	5102	4924	4755	4593	4496	4438	4291	4150	4015
K_V	182.32	158.16	138.54	121.19	105.89	92.02	84.36	80.14	69.62	60.68	52.47
μ_V	87.88	79.08	71.55	64.56	58.63	53.56	50.35	48.67	44.47	40.5	36.87
K_R	182.32	158.16	138.54	121.19	105.89	92.02	84.36	80.14	69.62	60.68	52.47
μ_R	82.64	76.66	70.90	64.54	58.27	52.03	47.45	44.85	37.56	29.53	20.73
K_{VRH}	182.32	158.16	138.54	121.19	105.89	92.02	84.36	80.14	69.62	60.68	52.47
μ_{VRH}	85.26	77.87	71.23	64.55	58.45	52.8	48.9	46.76	41.02	35.02	28.8
E_{VRH}	221.29	200.68	182.42	164.45	148.1	132.96	122.94	117.44	102.86	88.1	73.04
υ_{VRH}	0.298	0.289	0.281	0.274	0.267	0.259	0.257	0.256	0.254	0.258	0.268
v_p	3.943	3.837	3.736	3.621	3.506	3.391	3.298	3.246	3.092	2.905	2.678
v_s	13.404	12.799	12.268	11.738	11.223	10.706	10.377	10.190	9.674	9.154	8.590