Supporting Information

Elastic and Hydrostatic Behaviour of a Zinc Dietary Supplement, Zinc Glycinate Hydrate

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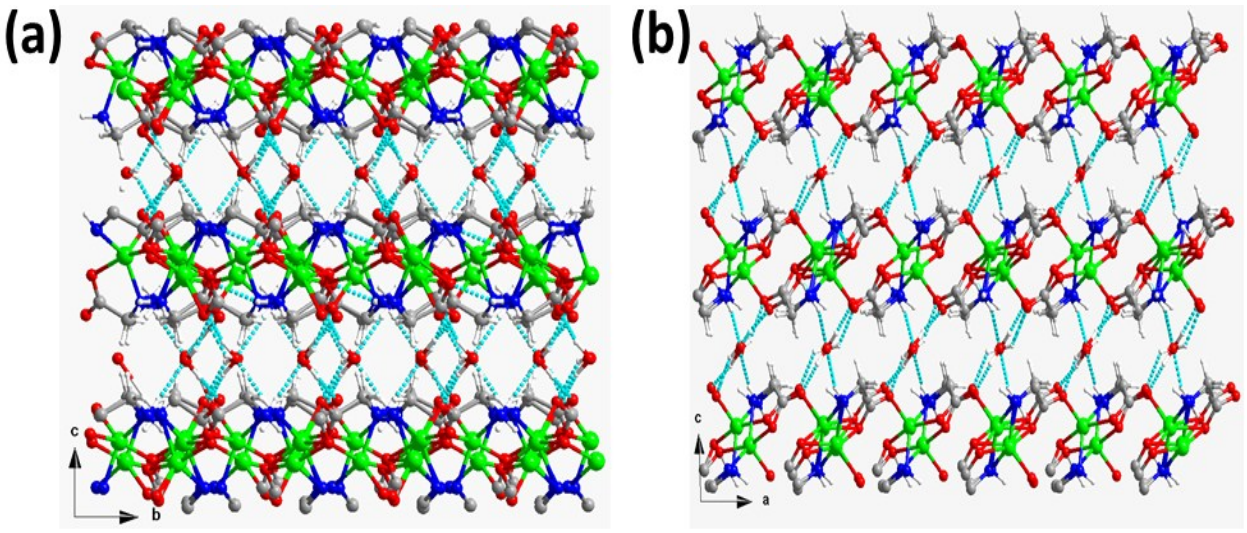

Fig. S1. Crystal structure of ZnG with hydrogen bonding. (a) View in ***bc***-plane (b) Layer stacking perpendicular to ***c***-axis view in ***ac***-plane.

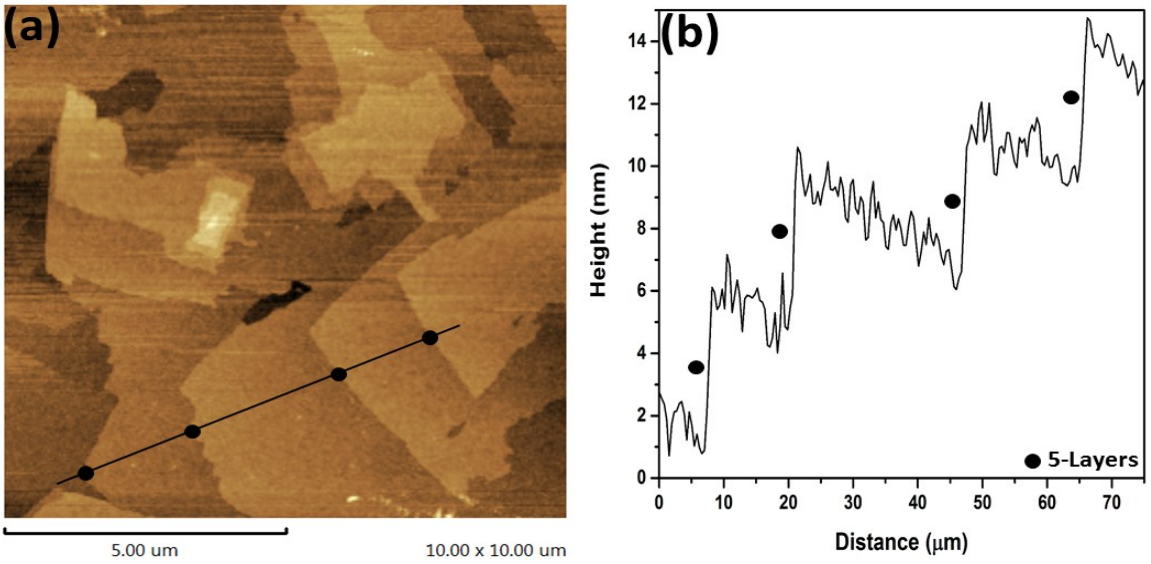

Fig. S2. The stacking and presence of layered nanosheets on the surface of the substrate at different places. (a) Stepwise stacking of layered nanosheets scanned at 5μm with area 10×10 μm^2. (b) Graphical representation of thickness of stacked nanosheets with height difference of ~4.2 nm correspond to 5-layers thickness.

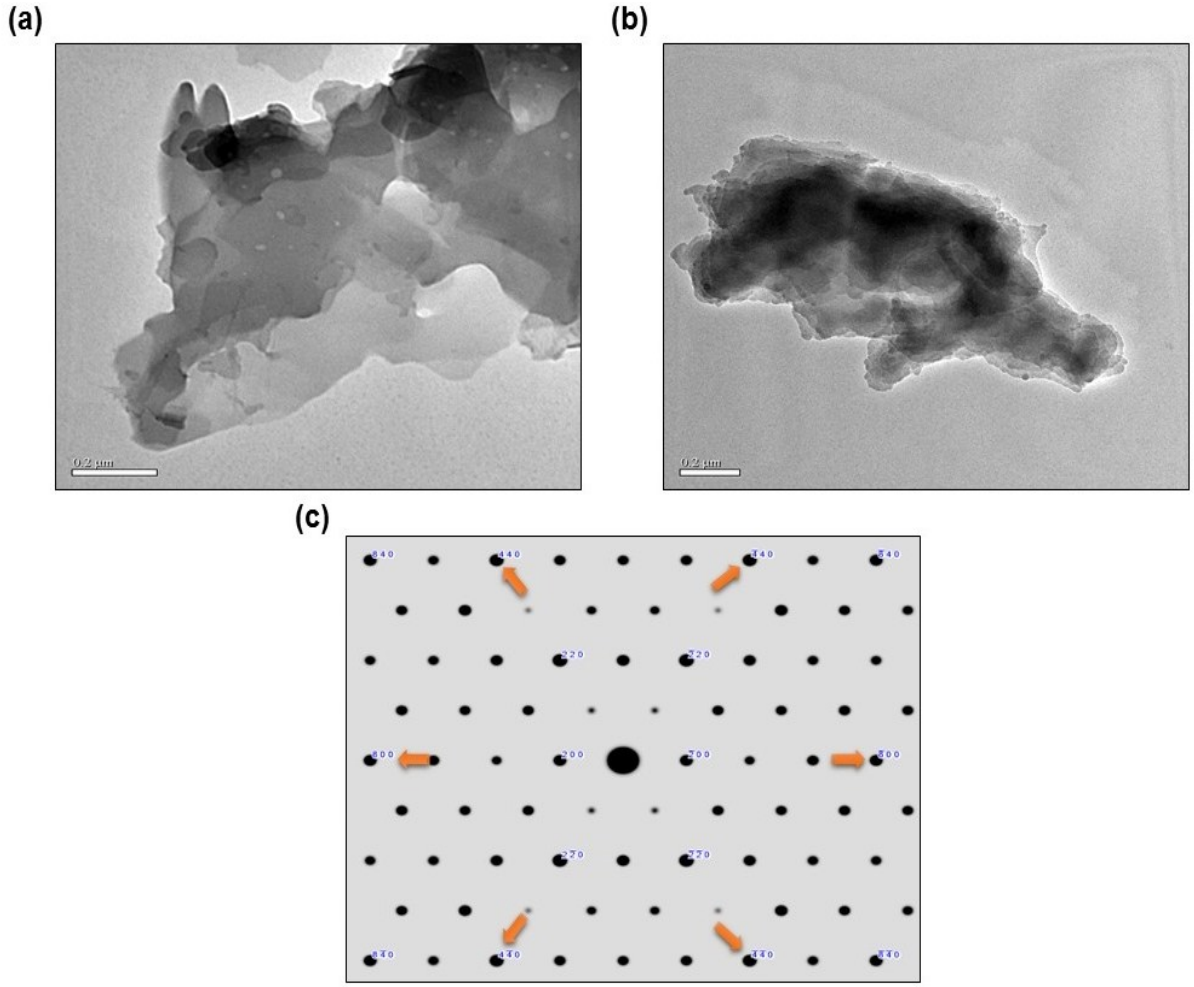

Fig. S3. TEM images of ZnG single crystal. (a-b) Bright field images of layered nanosheets with different lateral sizes. (c) Simulated diffraction pattern for mentioned planes along [001] direction.

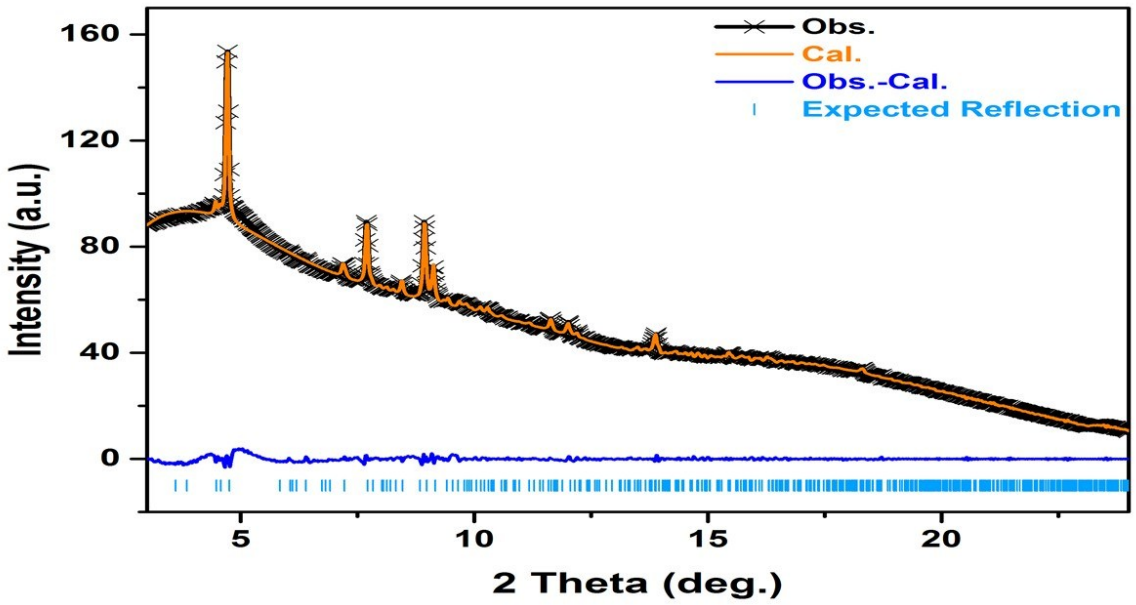

Fig. S4. The high-pressure synchrotron X-ray diffraction pattern of ZnG refined using Le Bail method to indicate its purity at ambient conditions. Black crosses: observed X-ray powder diffraction, Orange line: calculated profile; blue line: the difference between observed data and calculated profile. The light blue vertical markers indicate the allowed Bragg reflections. The final *Rp* and *Rwp* are 0.89% and 1.85%. The cell parameters were determined to be a = 19.714(2) Å, b = 10.468(13) Å, c = 15.048(15) Å, β = 92.806(2)°, V = 3109.28(13) Å^3

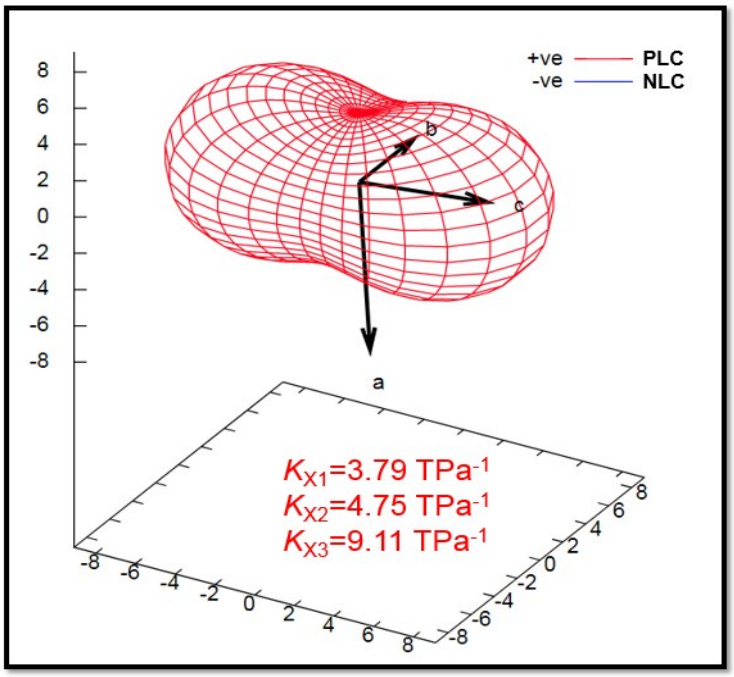

Fig. S5. The compressibility indicatrix for pressure range (ambient–12.10 GPa), while the magnitudes of corresponding compressibility K_{X1}, K_{X2} and K_{X3} are mentioned. The red values correspond to positive linear compressibility (PLC) and blue shows negative linear compressibility (NLC).

Table S1. The calculated 13 independent elastic constants.

Elastic constants												
***C*$_{ij}$(GPa)**												
C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{12}	C_{13}	C_{15}	C_{23}	C_{25}	C_{35}	C_{46}
66.85	54.09	26.59	12.19	16.12	14.75	28.42	23.38	14.17	23.80	1.42	3.51	-1.23

Table S2. The elastic moduli (E), Poisson's ratios (v) and shear moduli (G) extracted from the DFT calculation results.

Elastic modulus		Poisson's ratios				Shear modulus	
direction	**value**	**direction**	**value**	**direction**	**value**	**max**	**min**
x	36.11	xy	0.26	xz	0.54	19.15	6.52
y	30.61	yx	0.22	yz	0.73		
z	13.84	zx	0.20	zy	0.33		

Table S3. The calculated elastic moduli of ZnG under ambient pressure from first-principles calculations.

Orientation	Elastic Modulus (GPa)
[100]	36.11
~[010]	30.61
[001]	13.84

Table S4. Principal compressibilities and corresponding principal axes were determined using the PASCal software for ZnG.

Principal axis, *i*	K_{xi} (TPa^{-1})	Component of Xi along the crystallographic axes			Approximate axis
		a	***b***	***c***	
1	3.79	0.0834	0	0.9965	~[001]
2	4.75	0.0000	1	0.0000	[010]
3	9.11	-0.9964	0	0.0844	~[100]

Table S5. The experimental results of compressibility K_{X1}, K_{X2} and K_{X3} as a function of pressure.

Pressure (GPa)	Compressibility (TPa^{-1})		
	K_{X1}	K_{X2}	K_{X3}
0.00	----	----	----
1.32	10.37	3.64	3.24
4.6	9.42	4.32	3.64
5.39	9.31	4.46	3.69
6.23	9.21	4.59	3.74
7.24	9.11	4.75	3.79
9.38	8.94	5.05	3.88
10.87	8.84	5.25	3.93
12.1	8.77	5.4	3.97

Table S6. The calculated and experimental d-spacing for different crystalline planes.

Plane	Calculated (nm)	Experimental (nm)
(440)	0.2302	0.2068
$(\bar{4}\bar{4}0)$		
$(\bar{4}40)$	0.2302	0.1790
$(4\bar{4}0)$		
$(\bar{8}00)$	0.2459	0.2056
(800)		

Table S7. The lattice parameters of ZnG under different pressures extracted from HP-PXRD experiments.

P (GPa)	***a* (Å)**	***b* (Å)**	***c* (Å)**	***β***	***V* (Å^3)**
0	19.6641(38)	10.3681(22)	14.8933(27)	92.6534(39)	3033.2(10)
1.32	19.6450(31)	10.2897(19)	14.3974(20)	90.5897(41)	2910.1(8)
4.60	19.3281(42)	10.2002(24)	14.0071(28)	92.4180(50)	2759.0(10)
5.39	19.2191(17)	10.1668(07)	13.8861(11)	92.4044(33)	2710.9(3)
6.23	19.2068(36)	10.0844(18)	13.7650(24)	93.2365(76)	2661.9(8)
7.24	19.1086(52)	10.0394(33)	13.6508(42)	93.5490(99)	2613.7(13)
9.38	18.9082(59)	9.9486(36)	13.4371(45)	93.6660(82)	2522.5(14)
10.87	18.8377(52)	9.8424(27)	13.2249(36)	93.7157(84)	2446.8(11)
12.10	18.7174(35)	9.8087(22)	13.1143(29)	94.0106(95)	2401.8(8)