

Supporting Information

Mechanical Robustness in Fused Polyhedral Borane Crystals through Persistent Weak Intermolecular Interactions

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Experimental section

SC-XRD (Face Indexing)

SC-XRD data collection of $B_{18}H_{22}$ clusters was performed with a Bruker D8 VENTURE single-crystal X-ray diffractometer equipped with a graphite monochromatic Mo ($K\alpha$) ($\lambda = 0.71073 \text{ \AA}$) radiation and a PHOTON 100 CMOS detector. The data collection for both crystals was performed at 298 K. Face indexing was carried out by capturing a video of the crystals on the goniometer, and the faces were indexed using APEX-6 software.

CCDC number: 2265132 (*syn*- $B_{18}H_{22}$) and 602765(*anti*- $B_{18}H_{22}$).

Attenuated Total Reflectance Infrared Spectroscopy

A PerkinElmer attenuated total reflectance infrared (ATR-IR) spectrometer was used to analyse the crystalline samples.

Nanoindentation Measurements

The nanomechanical investigation of molecular crystals was conducted utilizing a Hysitron TI Premier Triboindenter system, equipped with a three-sided pyramidal Berkovich diamond indenter possessing a tip radius of 150 nm. Prior to experimental measurements, instrument calibration was performed through reference indents on a standardized fused quartz substrate, ensuring measurement traceability and system compliance correction. The *syn*- and *anti*-isomers of $B_{18}H_{22}$ single crystals were glued by Fevi-kwik on glass slides and directly subjected to nanoindentation without additional processing. Two primary testing methodologies were employed: load-controlled and displacement-controlled protocols. Load-controlled experiments implemented a trapezoidal waveform profile with peak loads of 1 mN and 5 mN, selected for their capacity to probe both near-surface and bulk mechanical response while maintaining quasi-static loading conditions. The trapezoidal function's linear loading segment (typically 5 second duration) enables controlled strain rate application, minimizing dynamic artefacts during plastic yield initiation. Complementary displacement-controlled testing prescribed maximum penetration depths of 300 nm and 600 nm to systematically investigate size-dependent mechanical behavior and substrate interaction effects in layered crystal systems.

Given the viscoelastic nature and enhanced ductility characteristic of molecular crystals relative to metallic/ceramic systems, time-dependent deformation analyses were integral to the

experimental matrix. Creep compliance was quantified through imposed 50s dwell periods at peak load, allowing stress relaxation kinetics to approach steady-state conditions before unloading. Concurrently, stress relaxation tests maintained constant displacement while monitoring load decay over equivalent durations, providing complementary data on molecular rearrangement kinetics under constrained deformation.

The unloading phase in the trapezoidal function is used to extract the elastic properties of the material by using gradual unloading of the nanoindenter from the sample. This gives an accurate load–displacement curve, which is important for analysing the material’s elastic modulus. Statistical analysis with all the data points also ensures that the data obtained are reproducible across multiple tests, making comparisons more reliable.

Nano Dynamic Mechanical Analysis Measurements

Dynamic mechanical analysis (DMA) was performed under a load-controlled frequency sweep mode. An oscillating dynamic load of 10 μN was applied on top of a static load of 1000 μN over a frequency range of 20–200 Hz. Also, the crystals are investigated with two different DMA load functions, viz., constant strain rate CMX (continuous measurement of X, X = hardness modulus, etc.) and linear CMX with peak loads of 1000 μN and 5000 μN . The storage modulus, loss modulus, and damping factors were determined by applying a sinusoidal force signal and recording the resulting displacement response.

Energy Frameworks Calculations: Energy frameworks calculations pertaining to intermolecular interactions were performed using the software suite Crystal Explorer ^{1,2} based on Gaussian B3LYP/6-31G(d,p) molecular wave-functions calculated using cif files of the crystals. Pairwise interaction energies between molecules were calculated considering a radius of 3.8 Å from centroid of a molecule to an atom (of another molecule) belonging to its nearest neighbour. The “energy framework” was constructed based on the crystal symmetry and total intermolecular interaction energy (E_{tot}), which includes electrostatic (E_{ele}), polarization (E_{pol}), dispersion (E_{dis}), and exchange-repulsion components (E_{rep}) with scale factors of 1.057, 0.740, 0.871 and 0.618 respectively. Where $E_{\text{total}} = 1.057E_{\text{ele}} + 0.740E_{\text{pol}} + 0.871E_{\text{dis}} + 0.618 E_{\text{rep}}$. The analysis was carried out based on their respective crystal geometries. The X-H bond lengths are normalised by Crystal Explorer to be the same as those obtained from neutron diffraction experiments.³ The energy cut-off was kept to 10 kJ/mol for all the systems while evaluating the total interaction energies.

Computational Details

The elastic properties of borane clusters ($B_{18}H_{22}$) were investigated using plane-wave density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) (Kresse & Hafner, 1994).^{4,6} Projector-augmented wave (PAW) pseudopotentials were employed to approximate the frozen-core electrons of various elements. The exchange-correlation functional was described using the Perdew–Burke–Ernzerhof (PBE) (Kresse & Furthmüller, 1996; Kresse & Joubert, 1999)^{7,8} formulation within the generalized gradient approximation (GGA) (Perdew et al., 1996),⁹ with additional dispersion corrections incorporated via the Tkatchenko–Scheffler pairwise correction method (Tkatchenko & Scheffler, 2009).¹⁰ A Gaussian smearing width of 0.05 eV and a plane-wave energy cutoff of 500 eV were applied. The k-point mesh width was set to $0.33 \text{ \AA}^{-1}$, determined through convergence tests on elastic constants and ground-state energy.

The strain energy has been expressed as function of applied strains for the quantification the elastic constants for the materials that follow Hooke’s law in elastic region:

$$E(V, \epsilon) = E(V_0, \epsilon=0) + V_0 \left(\sum_{i,j=1}^3 \sigma_{ij} \epsilon_{ij} + \frac{1}{2} \sum_{i,j=1}^3 C_{ijkl} \epsilon_{ij} \epsilon_{kl} \right) + \dots \quad (1)$$

where, V_0 is the equilibrium volume fo the undeformed crystal lattice. C_{ijkl} is a forth order stiffness tensor and ϵ_{ij} represents the strain components. The stiffness tensor is simplified using Voigt notation (C_{ij}), derived from the second derivative of the total energy with respect to strain ($C_{ij} = \frac{1}{V_0} \frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j}$). ϵ_i is the Voigt strain having six components. The elastic constants are determined by applying controlled strain tensors to the simulation cell and solving the resulting energy-strain equations, leveraging crystal symmetry to reduce the number of independent constants. *syn*- $B_{18}H_{22}$ (monoclinic structure), 13 independent elastic constants are required whereas *anti*- $B_{18}H_{22}$ (Orthorhombic structure) exhibits only 9 due to higher symmetry. This symmetry-driven reduction enables efficient computation of anisotropic elastic behavior in boron hydride systems.

In each case, controlled strains (δ) are applied within the elastic limit ($\pm 3\% \sim \pm 10\%$), and the resulting energy-strain relationship is fitted to a quadratic polynomial $ax^2 + bx + c$. The second-order coefficient a corresponds to combinations of elastic constants (Table 1). By solving the system of equations derived from these coefficients, the independent elastic constants are obtained. This approach accounts for symmetry-driven reductions in complexity while

ensuring computational precision. The details of computational information has been documented in github ([GitHub - prnvrvs/elastic_vasp](https://github.com/prnvrvs/elastic_vasp)) and in (Kumar & Adlakha, 2023).¹¹

Nanoindentation:

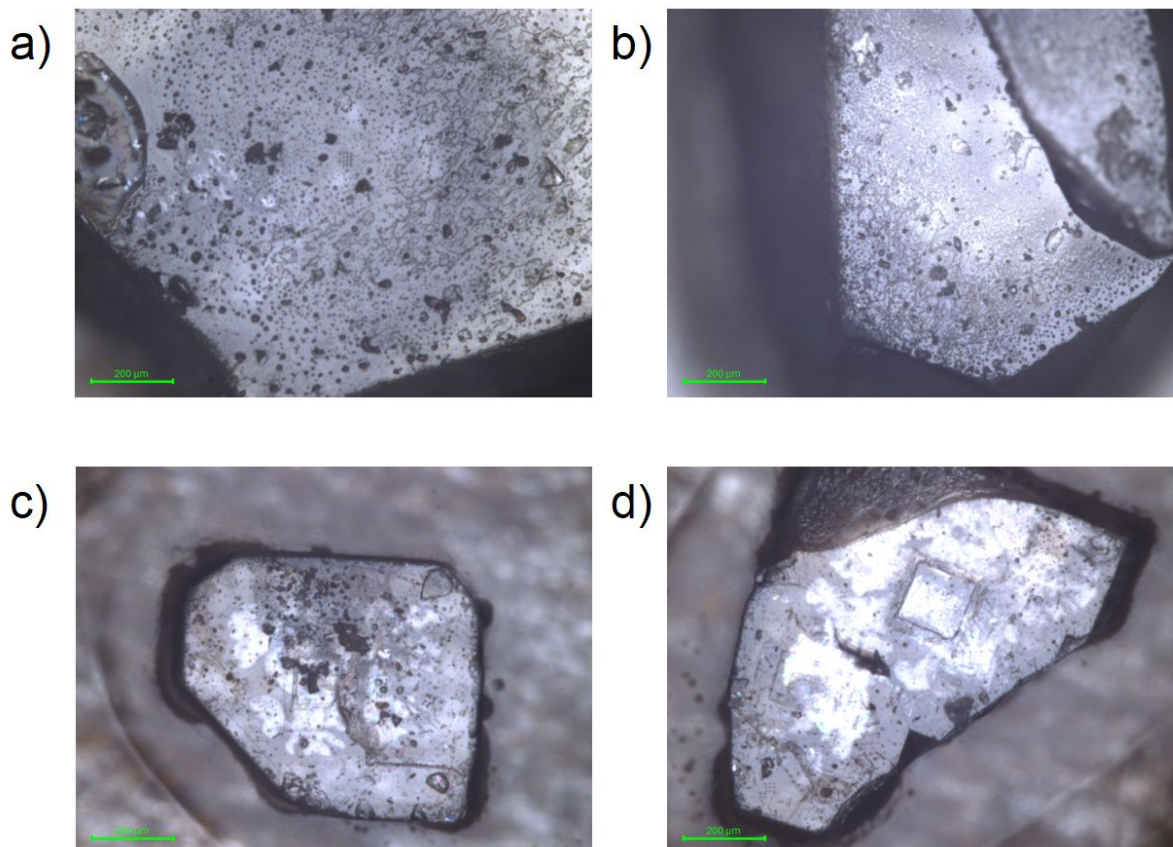


Figure S1. Optical images of the crystals on which NI experiments were performed. The upper panel represents *syn*-B₁₈H₂₂ crystals (a & b), and the lower panel represents *anti*-B₁₈H₂₂ crystals (c & d).

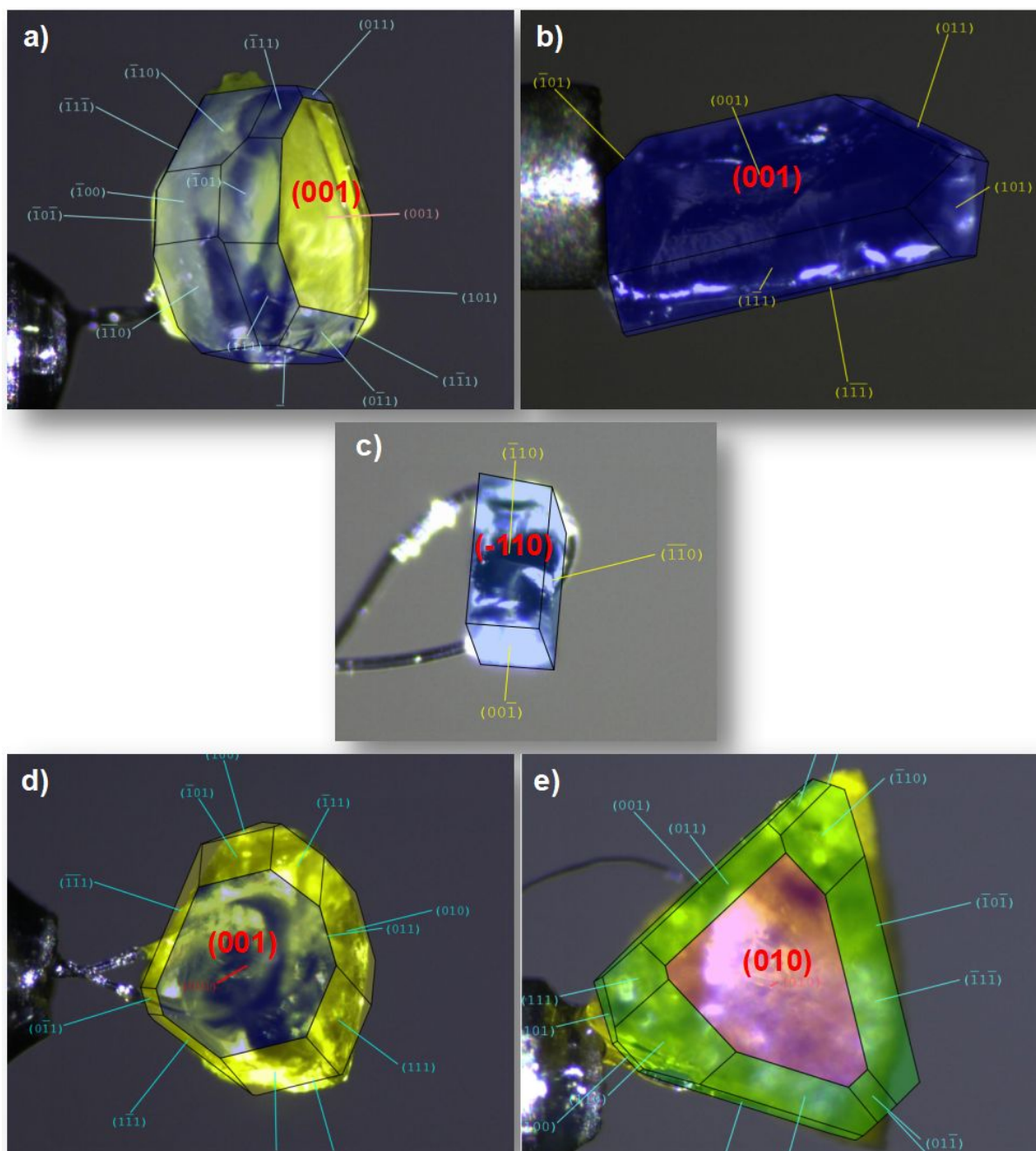


Figure S2: Face indexing of a) *syn*-B₁₈H₂₂, b) and *anti*-B₁₈H₂₂, c) B₁₀H₁₄, d) 4-HS-B₁₈H₂₁, and e) HS-B₁₀H₁₃. The major face, where nanoindentation was performed, is highlighted in red.

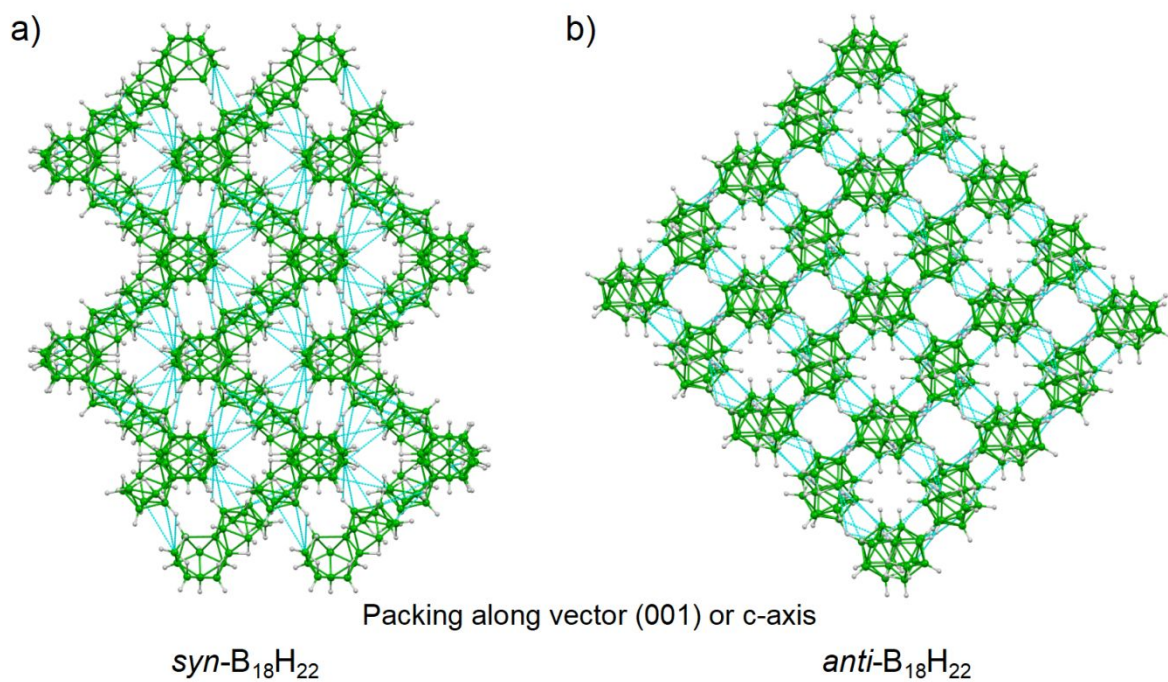


Figure S3: Supramolecular packing with short contacts of *syn*-B₁₈H₂₂ (a) and *anti*-B₁₈H₂₂ (b) along c-axis.

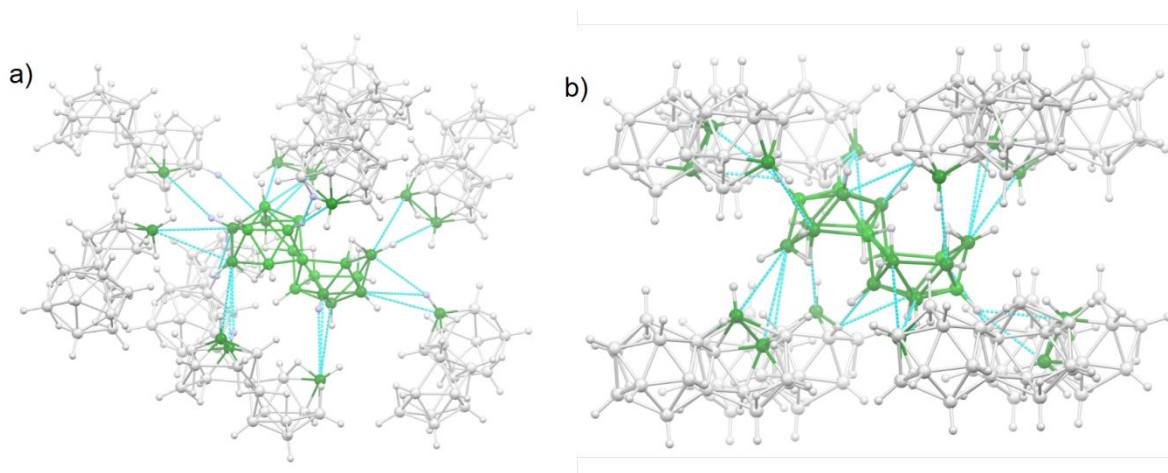


Figure S4: Short contacts showing each molecule of *syn*-B₁₈H₂₂ (a) and *anti*-B₁₈H₂₂ (b) are connected to eight neighbouring molecules, respectively.

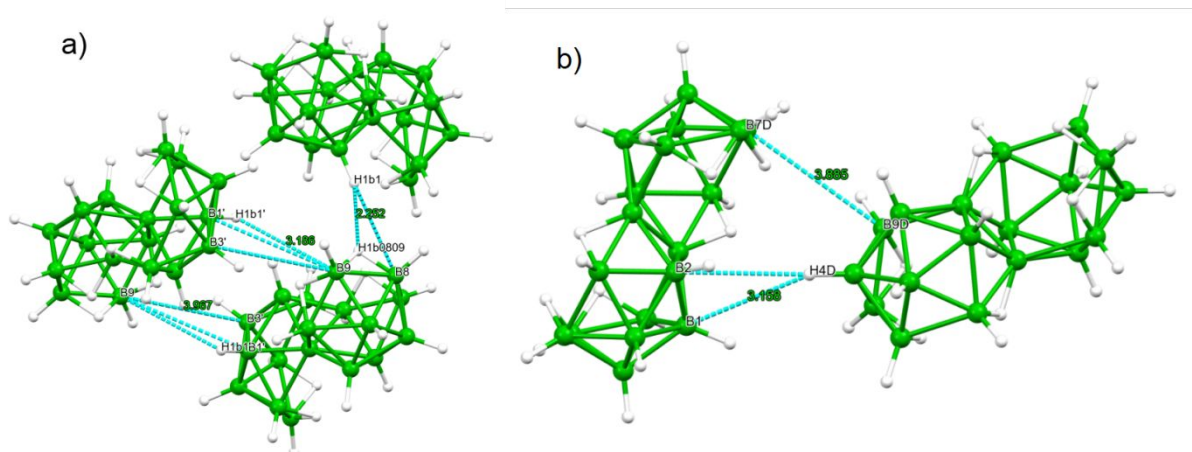


Figure S5. Short contacts distances of B $\cdots\mu$ -BHB, B-H $\cdots$ B, and B $\cdots$ B interactions in *syn*-B₁₈H₂₂ (a) and *anti*-B₁₈H₂₂ (b).

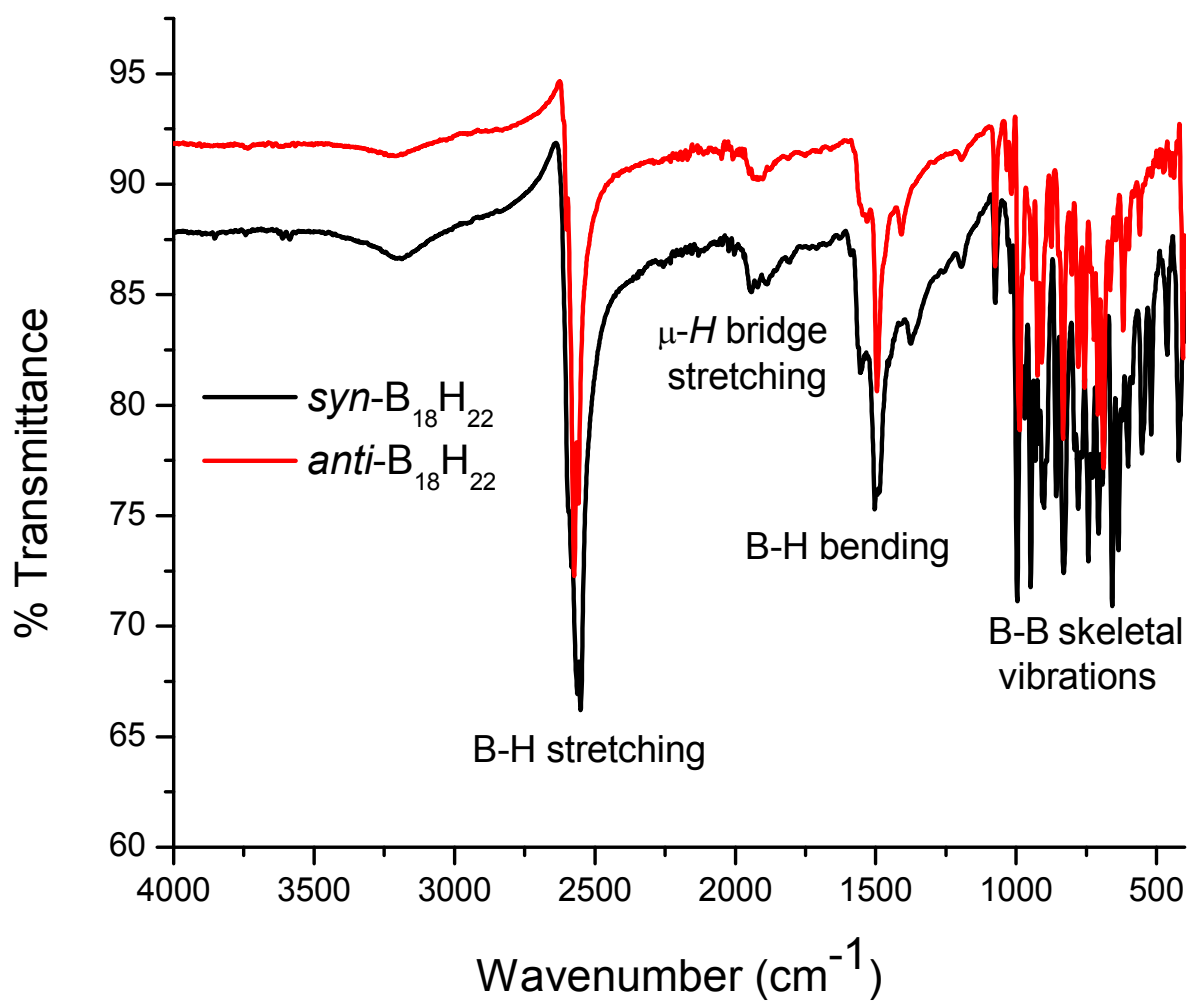


Figure S6: ATR-IR of *syn*-B₁₈H₂₂ and *anti*-B₁₈H₂₂.

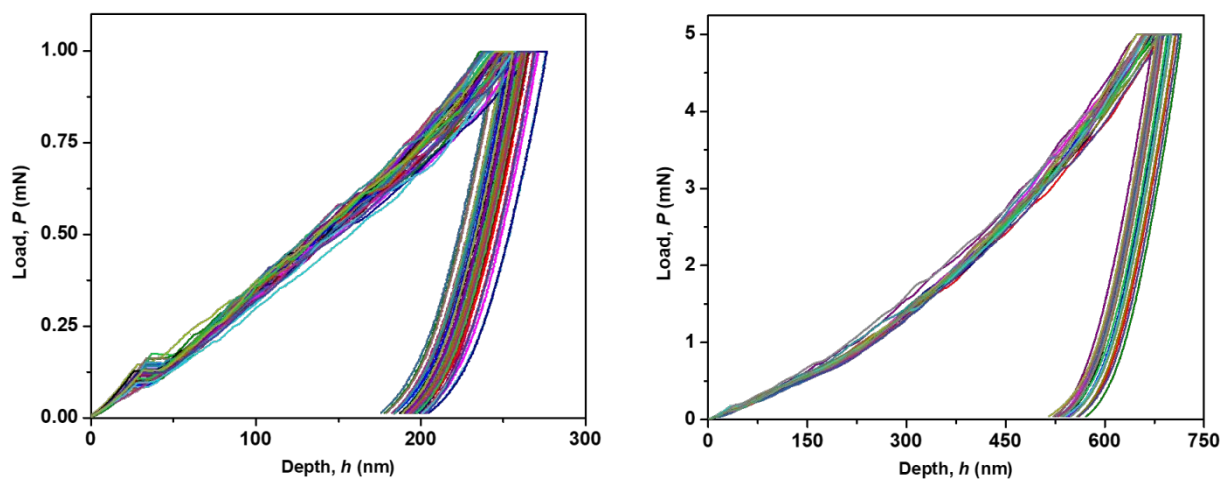


Figure S7. Multiple P-h curves at 1mN and 5mN loads for *syn*-B₁₈H₂₂.

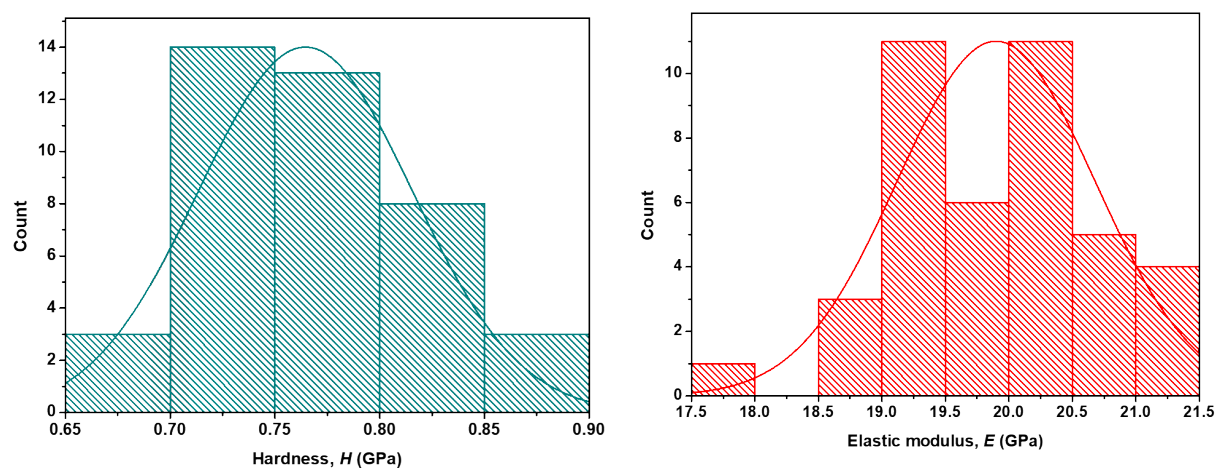


Figure S8. Histogram plots of H & E at 1mN load for *syn*-B₁₈H₂₂.

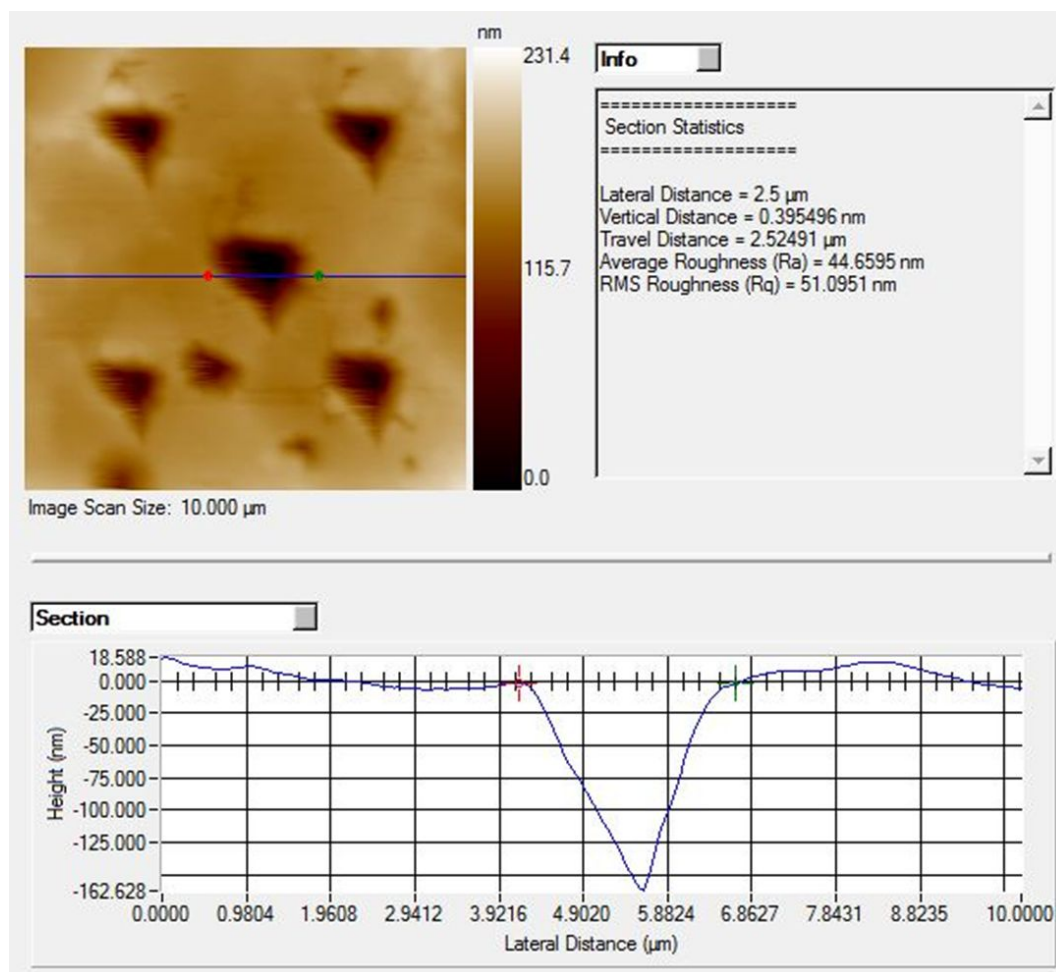


Figure S9. Height profile of the indent impression of *syn*-B₁₈H₂₂ at 1mN load.

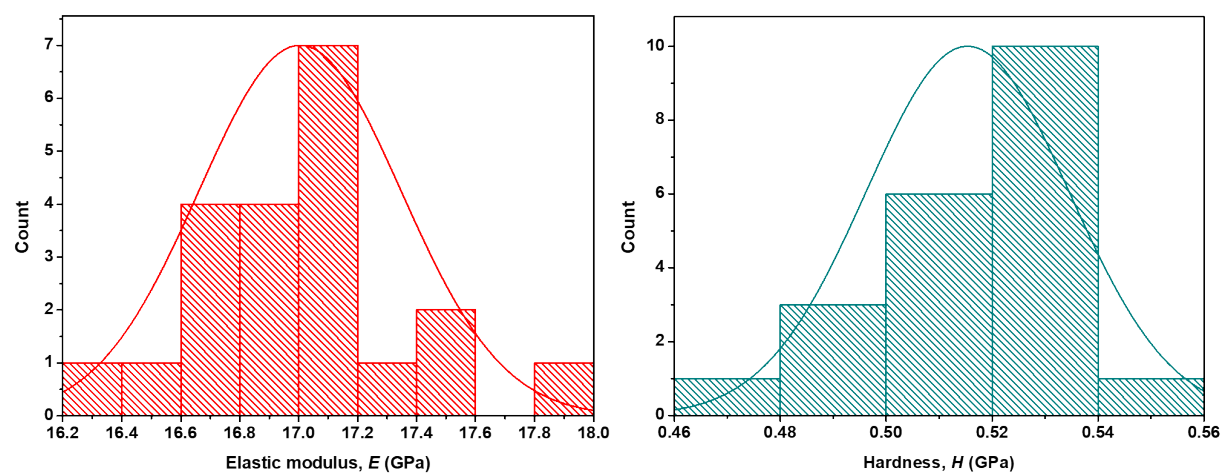


Figure S10. Histogram plots of H & E at 5mN load for *syn*-B₁₈H₂₂.

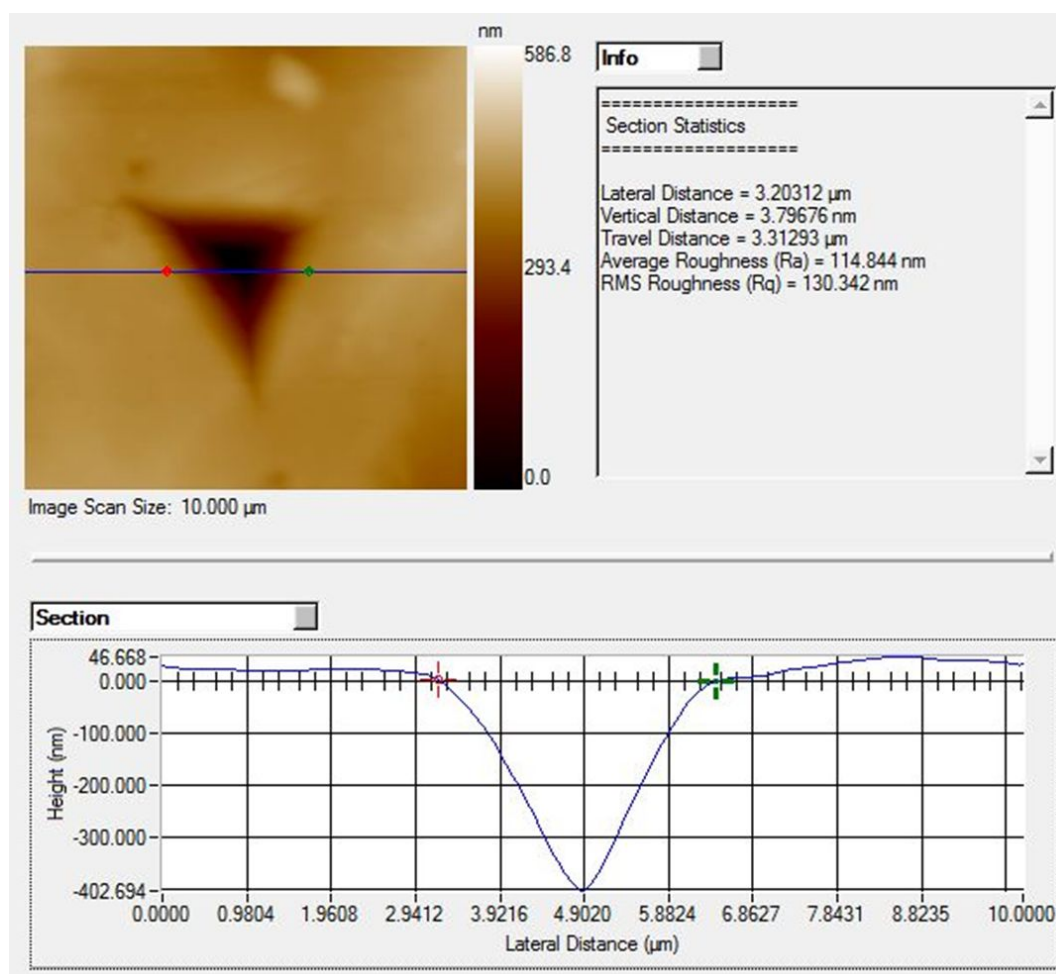


Figure S11. Height profile of the indent impression of *syn*-B₁₈H₂₂ at 5 mN load.

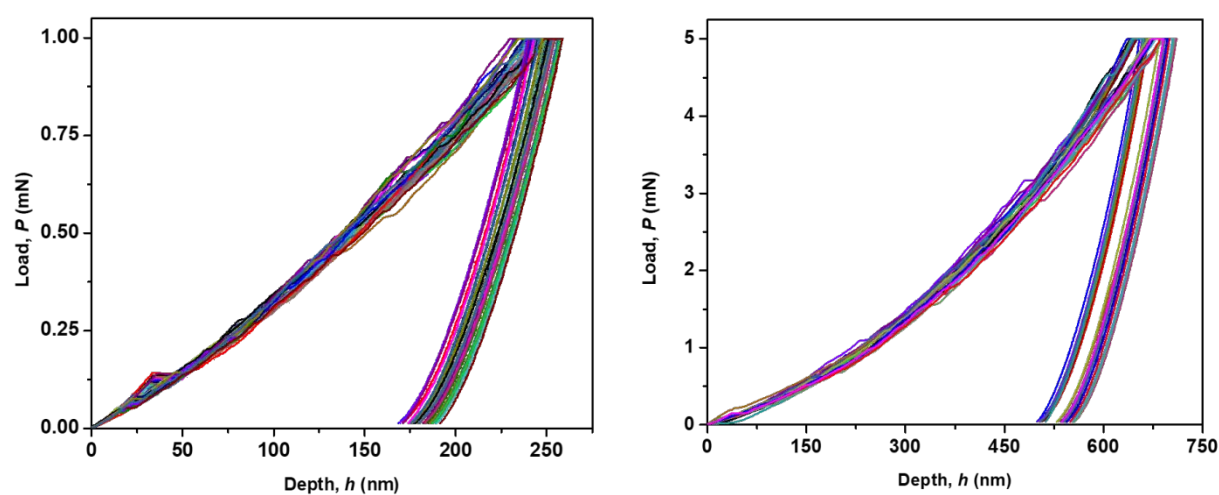


Figure S12. Multiple P-h curves at 1 mN and 5 mN loads for *anti*-B₁₈H₂₂.

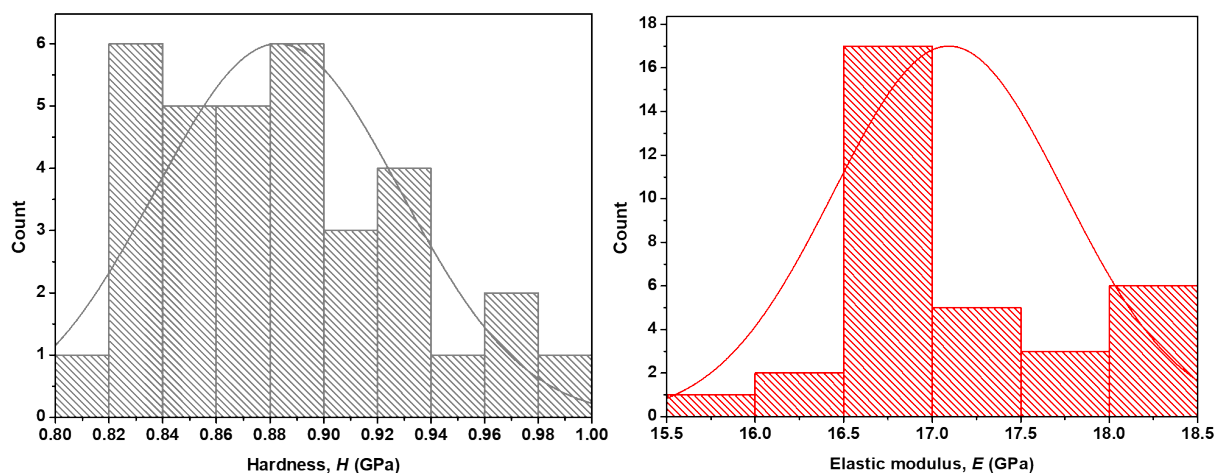


Figure S13. Histogram plots of H & E at 1mN load for *anti*-B₁₈H₂₂.

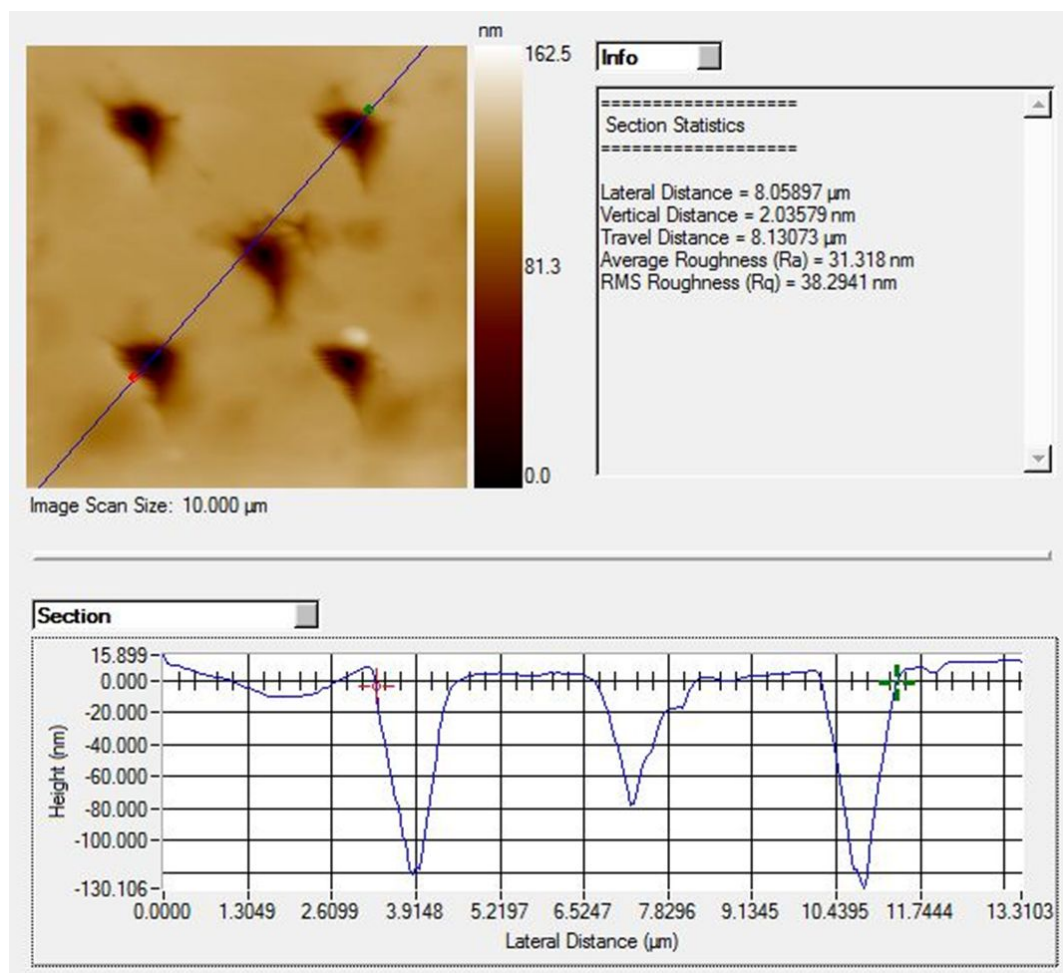


Figure S14. Height profile of the indent impression of *anti*-B₁₈H₂₂ at 1mN load.

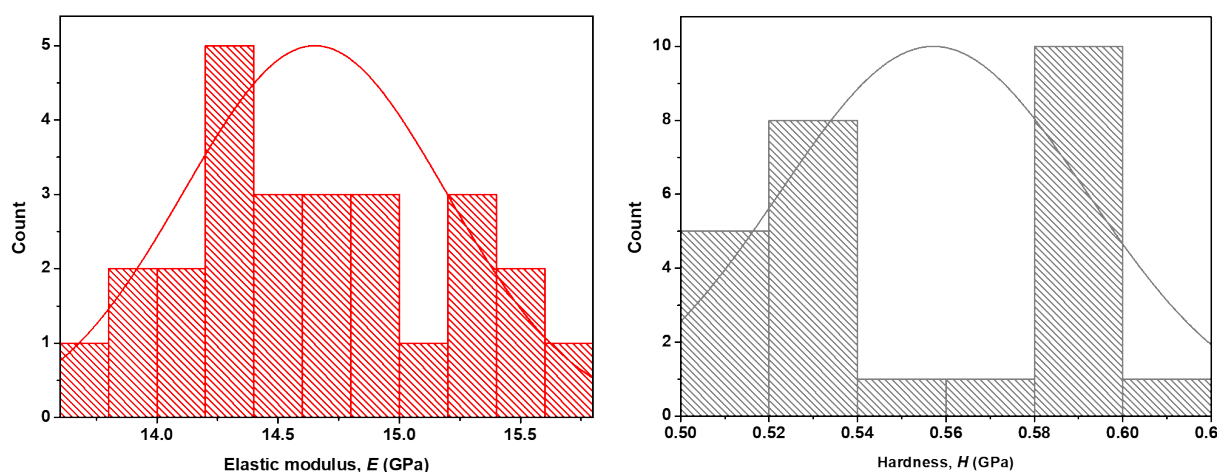


Figure S15. Histogram plots of H & E at 5mN load for *anti*-B₁₈H₂₂.

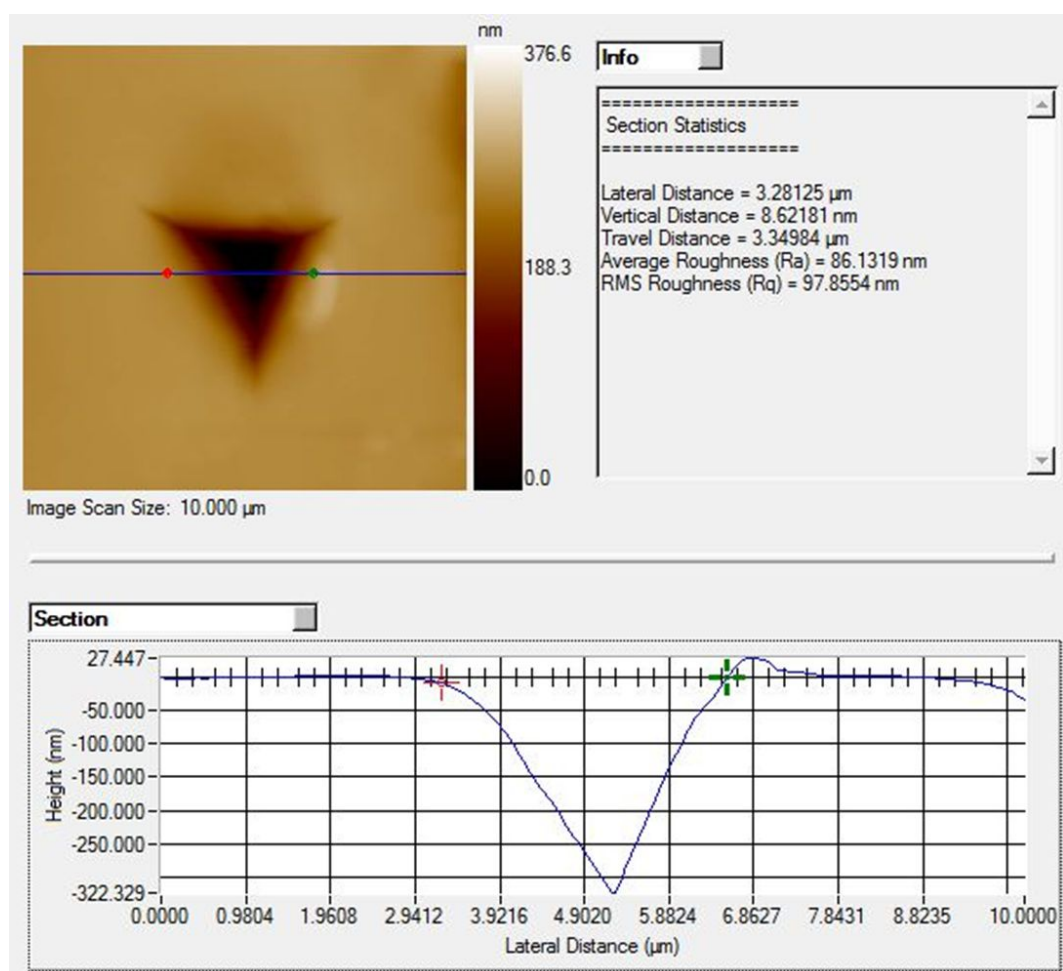


Figure S16. Height profile of the indent impression of *anti*-B₁₈H₂₂ at 5mN load.

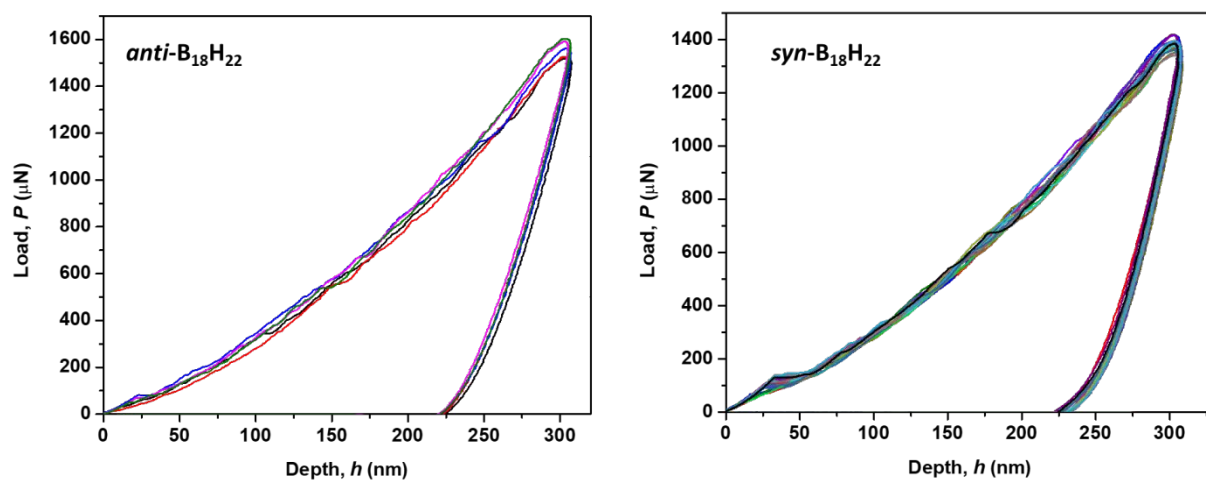


Figure S17. Depth-controlled multiple P-h curves at 300nm displacement for both the *syn*- & *anti*-B₁₈H₂₂ crystals.

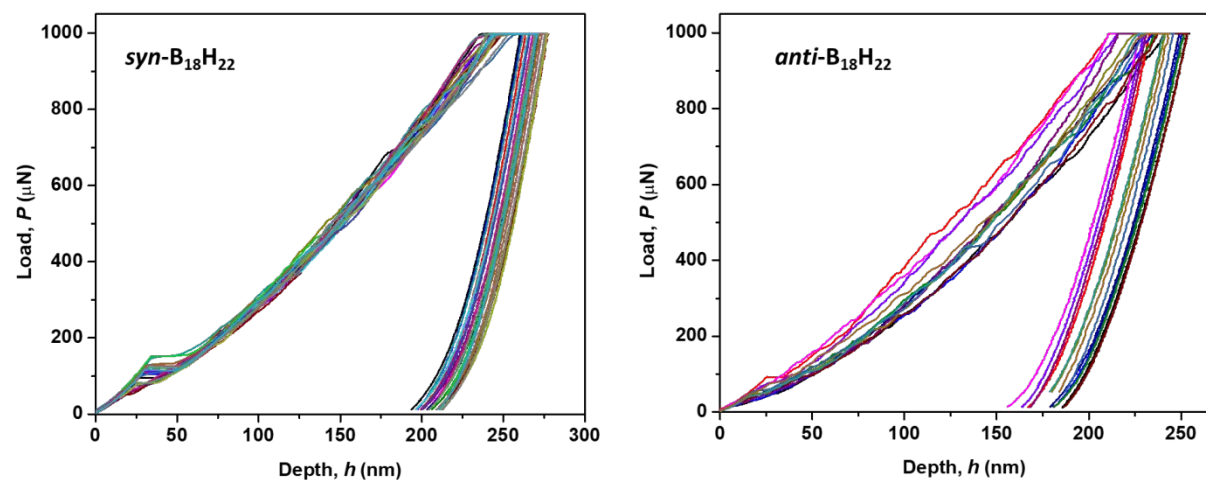


Figure S18. Multiple P-h curves obtained from the creep test with 1mN peak load and 5-50-5 s & 1-30-1 s load functions for the *syn* & *anti*-B₁₈H₂₂ crystals.

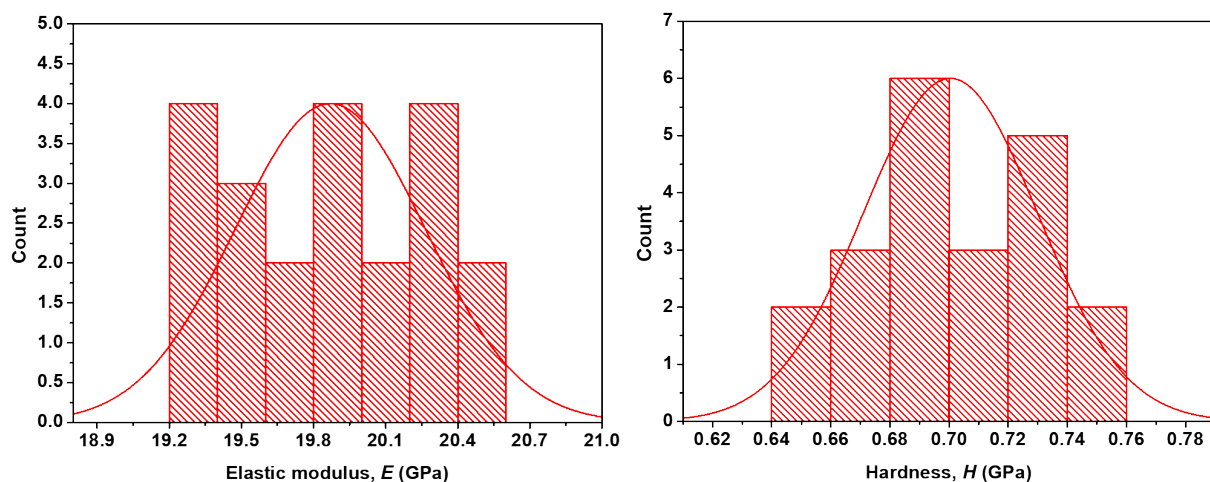


Figure S19. Histogram plots of H & E obtained from creep test at 1mN load for *syn*-B₁₈H₂₂.

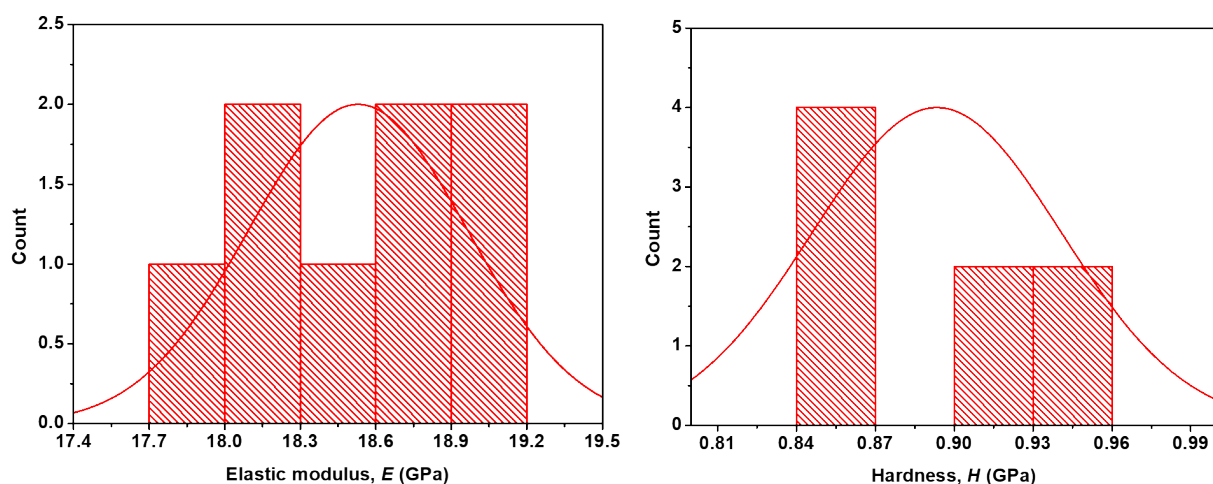


Figure S20. Histogram plots of H & E obtained from creep test at 1mN load for *anti*-B₁₈H₂₂.

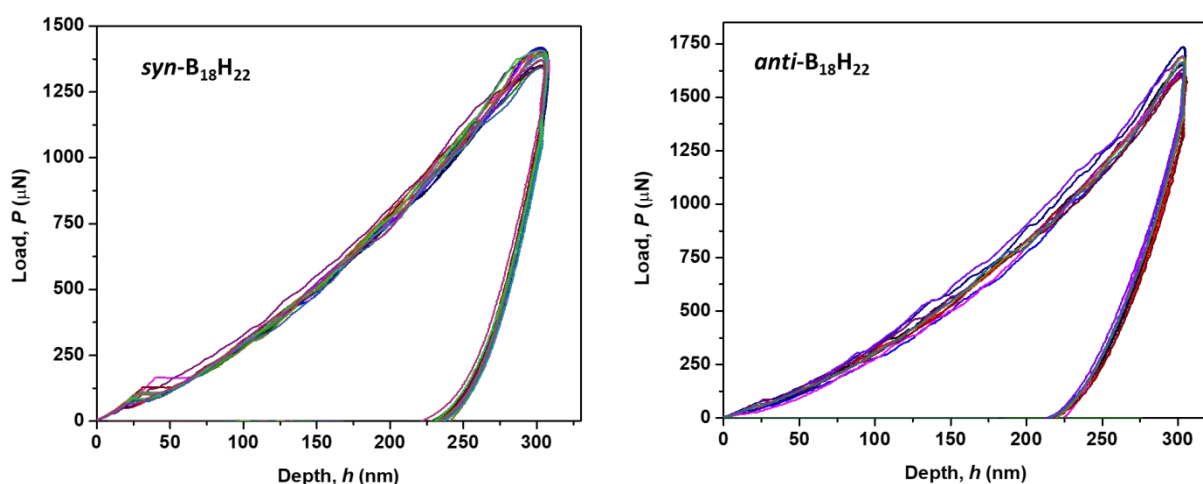


Figure S21. Multiple P - h curves obtained from the stress relaxation test with 300nm indenter displacement and 5-50-5 s & 1-30-1 s load functions for the *syn*- & *anti*-B₁₈H₂₂ crystals.

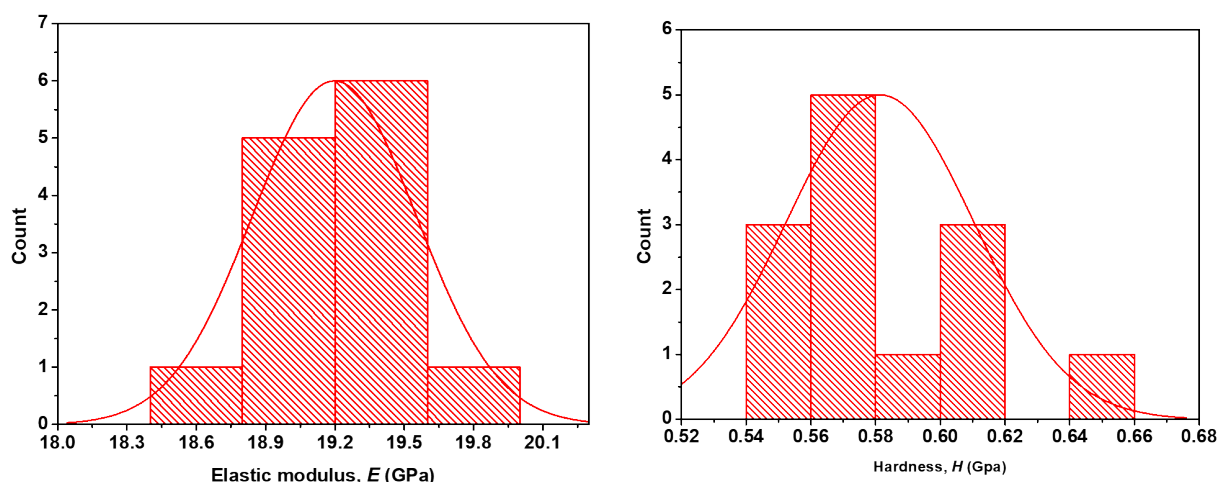


Figure S22. Histogram plots of H & E obtained from stress relaxation test at 300nm fixed indenter displacement for *syn*-B₁₈H₂₂.

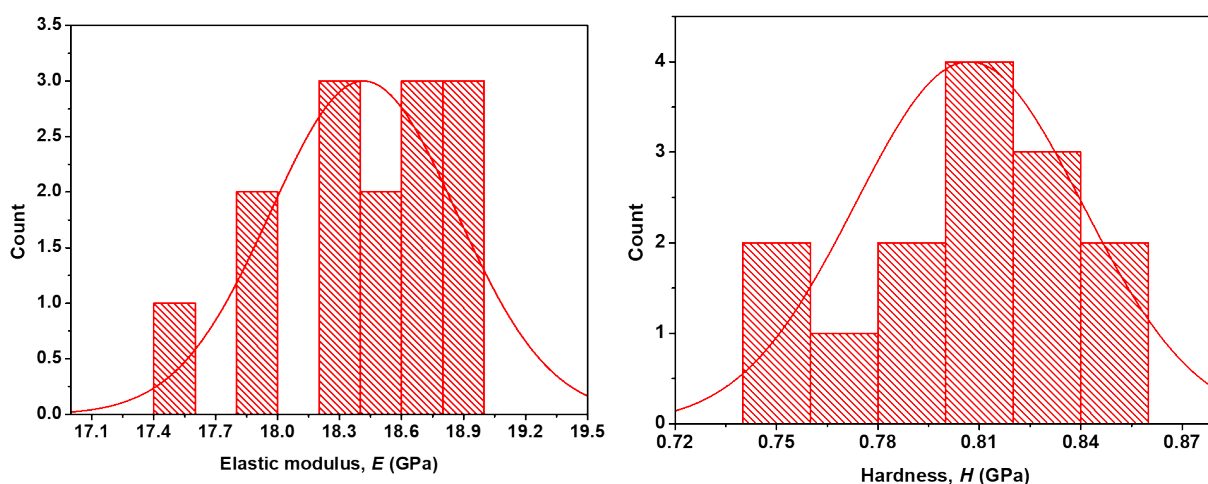


Figure S23. Histogram plots of H & E obtained from stress relaxation test at 300nm fixed indenter displacement for *anti*-B₁₈H₂₂.

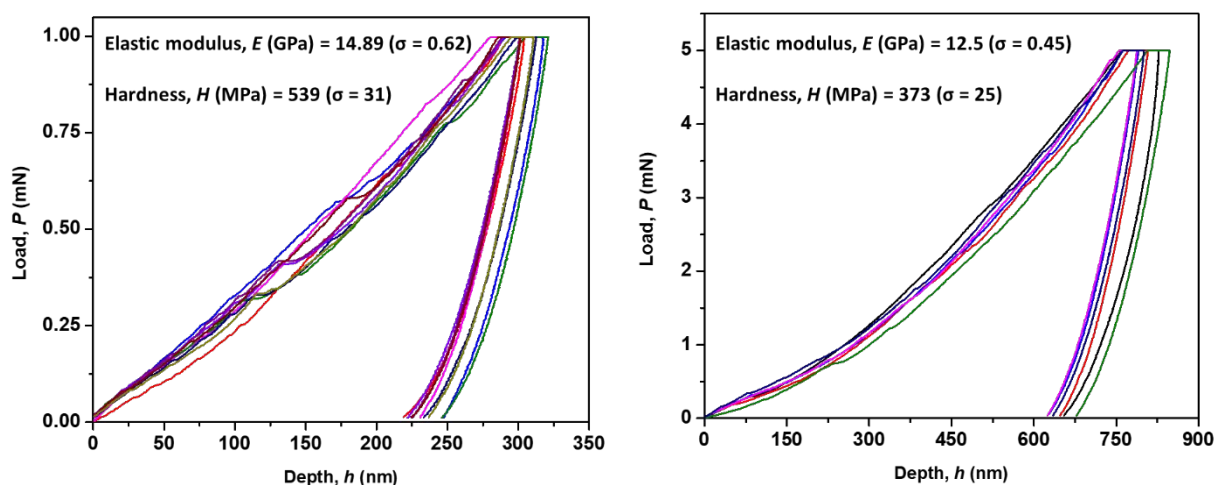


Figure S24. Multiple P - h curves and the H and E values of SH-*syn*-B₁₈H₂₁ at different loads.

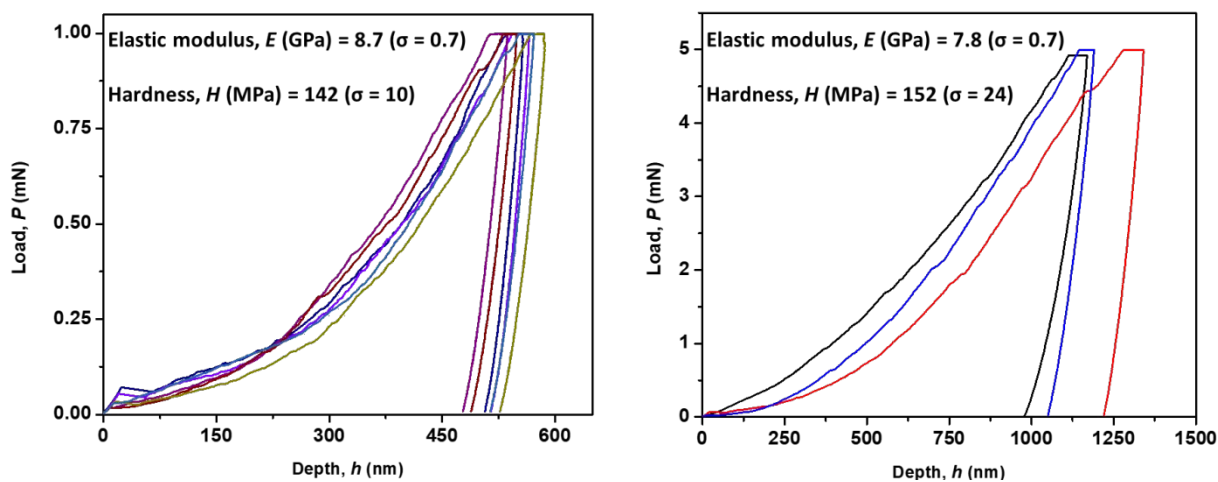


Figure S25. Multiple $P-h$ curves and the H and E values of $B_{10}H_{14}$ at different loads.

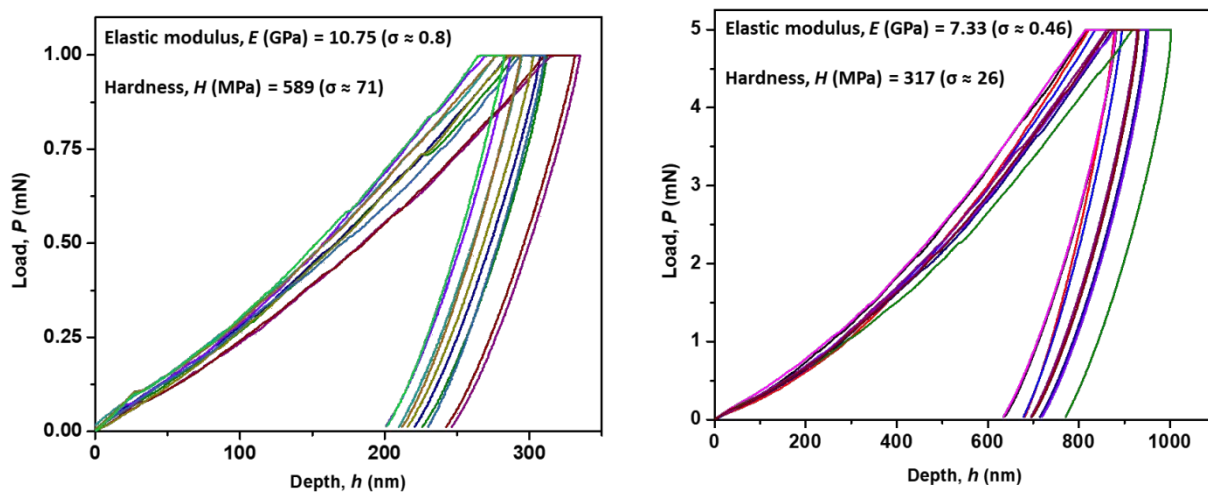


Figure S26. Multiple $P-h$ curves at two different loads (1 mN & 5 mN) and the H and E values of $SH-B_{10}H_{13}$.

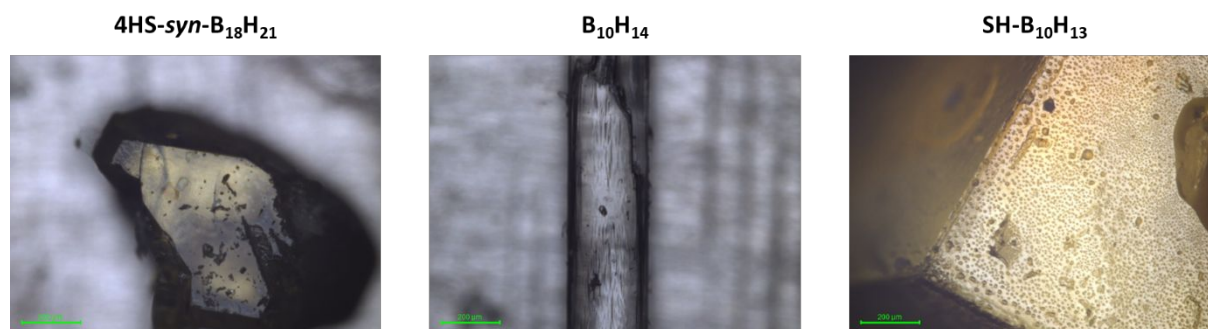


Figure S27. Optical images of SH-*syn*-B₁₈H₂₁, B₁₀H₁₄ and SH-B₁₀H₁₃ crystals on which nanoindentation experiments were carried out.

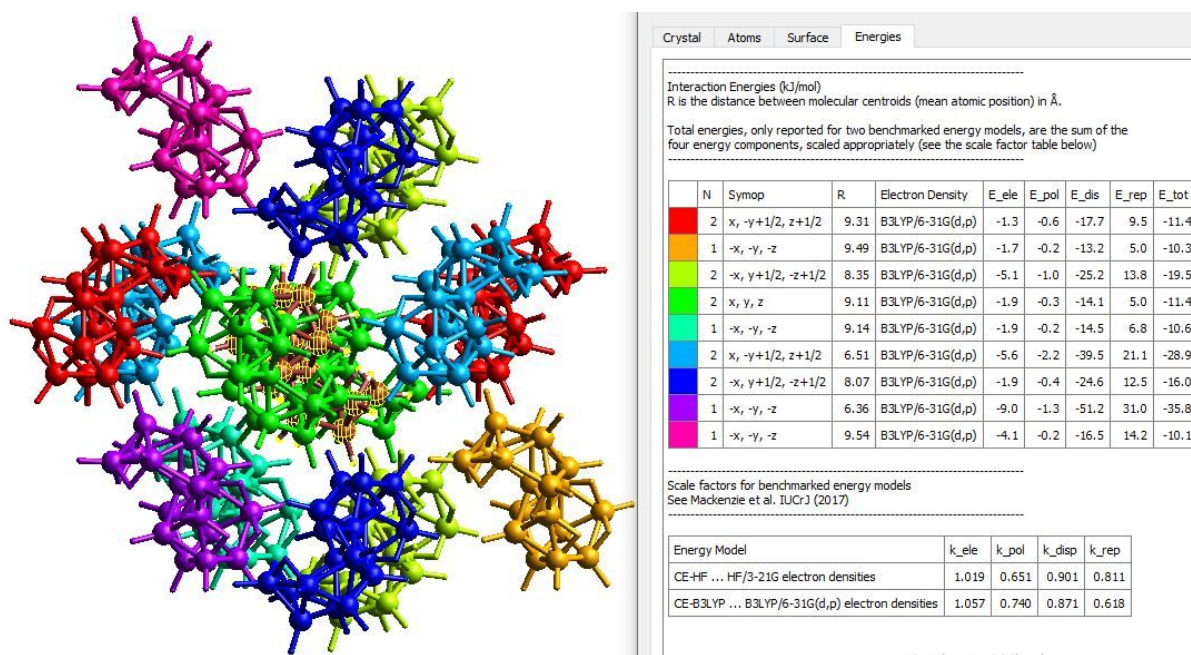


Figure S28. Energy frameworks calculations of *syn*-B₁₈H₂₂. The total interaction energy is -241.2 kJ/mol.

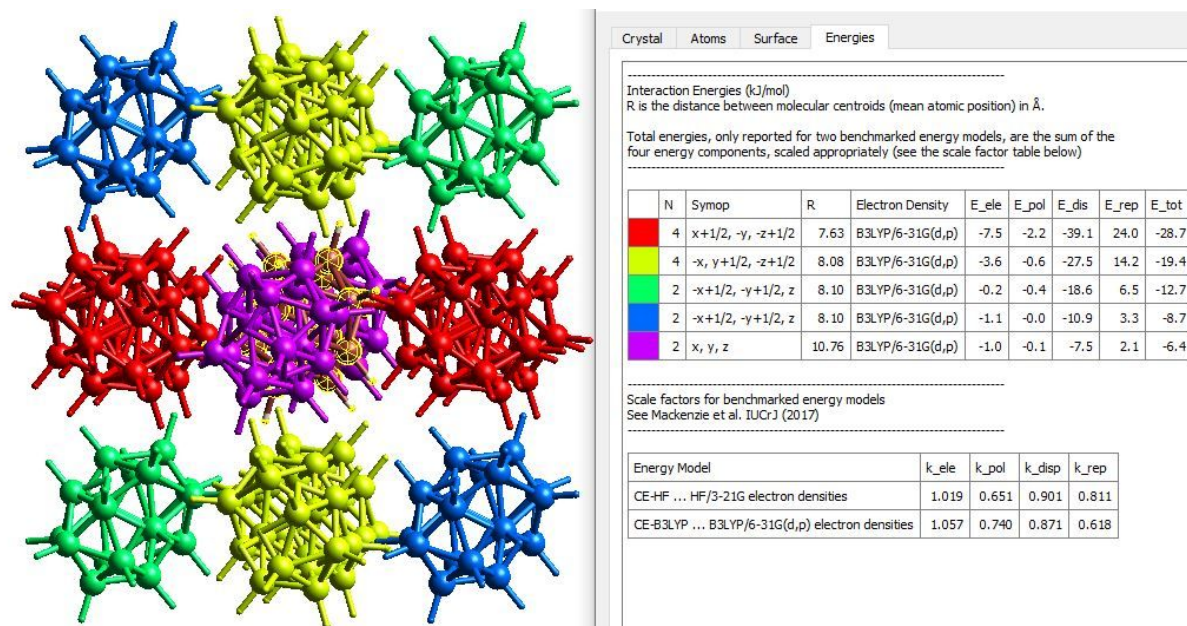


Figure S29. Energy frameworks calculations of *anti*-B₁₈H₂₂. The total interaction energy is -217.8 kJ/mol.

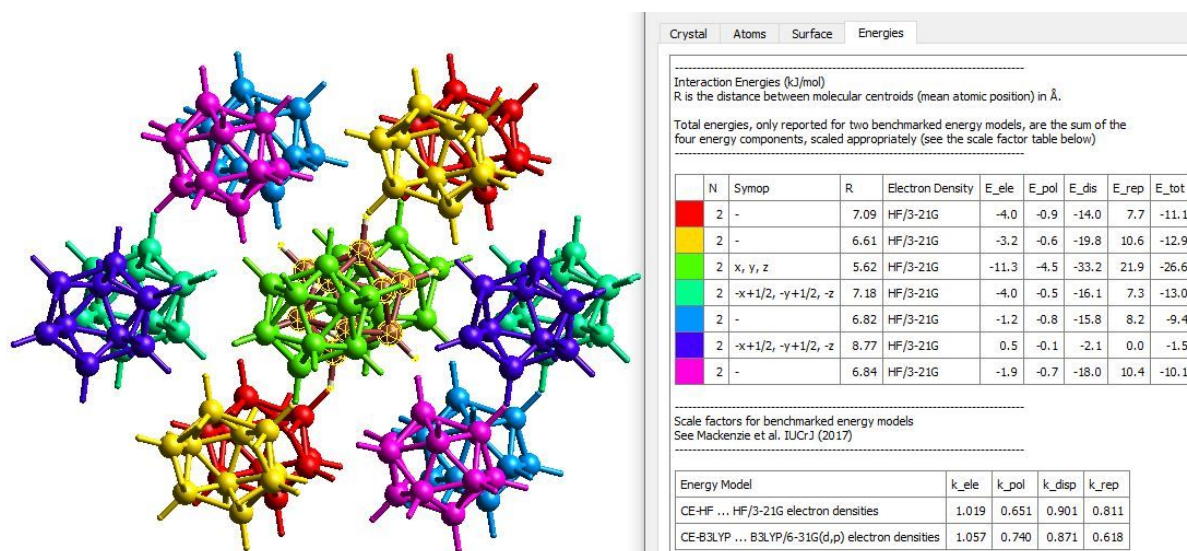


Figure S30. Energy frameworks calculations of B₁₀H₁₄. The total interaction energy is -154.2 kJ/mol.

Table S1: Various distortions imposed on the unit cell for different crystal symmetry.

Crystal	Symmetry	Imposed Strain
<i>syn</i>-B₁₈H₂₂	Monoclinic	$\left[\delta, -\delta, \frac{\delta^2}{(1-\delta^2)}, 0, 0, 0 \right]$ $[\delta, \delta, 0, 0, 0, 0]$ $\left[\frac{\delta^2}{(1-\delta^2)}, \delta, -\delta, 0, 0, 0 \right]$ $[0, \delta, \delta, 0, 0, 0]$ $\left[\delta, \frac{\delta^2}{(1-\delta^2)}, -\delta, 0, 0, 0 \right]$ $[\delta, 0, \delta, 0, 0, 0]$ $\left[\frac{\delta^2}{(4-\delta^2)}, 0, 0, \delta, 0, 0 \right]$ $[\delta, 0, 0, 0, \delta, 0]$ $[\delta, 0, 0, 0, -\delta, 0]$ $[0, \delta, 0, 0, \delta, 0]$ $[0, 0, \delta, 0, \delta, 0]$ $[0, 0, 0, \delta, 0, \delta]$ $[0, 0, 0, 0, \delta, -\delta]$
<i>anti</i>-B₁₈H₂₂	Orthorhombic	$[\delta, \delta, 0, 0, 0, 0]$ $\left[\delta, -\delta, \frac{\delta^2}{(1-\delta^2)}, 0, 0, 0 \right]$ $[\delta, 0, \delta, 0, 0, 0]$ $\left[\delta, \frac{\delta^2}{(1-\delta^2)}, -\delta, 0, 0, 0 \right]$ $[0, \delta, \delta, 0, 0, 0]$ $\left[\frac{\delta^2}{(1-\delta^2)}, \delta, -\delta, 0, 0, 0 \right]$ $[0, 0, 0, \delta, 0, 0]$ $[0, 0, 0, 0, \delta, 0]$ $[0, 0, 0, 0, 0, \delta]$

Table S2: Different modulus values (average) obtained from different Computational methods for *syn*-B₁₈H₂₂ and *anti*-B₁₈H₂₂

Method	Bulk (GPa)		Young (GPa)		Shear (GPa)	
	<i>syn</i> -B ₁₈ H ₂₂	<i>anti</i> -B ₁₈ H ₂₂	<i>syn</i> -B ₁₈ H ₂₂	<i>anti</i> -B ₁₈ H ₂₂	<i>syn</i> -B ₁₈ H ₂₂	<i>anti</i> -B ₁₈ H ₂₂
Voigt	17.826667	9.166667	33.101375	18.62034	13.902000	8.016
Reuss	17.683871	9.146312	30.513706	16.54388	12.583855	6.901723
Hill	17.755269	9.156489	31.818161	17.59812	13.242927	7.458862

$$\text{Elastic Constant (syn-B}_{18}\text{)} = \begin{bmatrix} 29.76 & 11.55 & 9.76 & 0 & -0.69 & 0 \\ 11.55 & 34.71 & 11.45 & 0 & 3.96 & 0 \\ 9.76 & 11.45 & 30.45 & 0 & -2.34 & 0 \\ 0 & 0 & 0 & 14.36 & 0 & -1.88 \\ -0.69 & 3.96 & -2.34 & 0 & 14.24 & 0 \\ 0 & 0 & 0 & -1.88 & 0 & 20.19 \end{bmatrix}$$

$$\text{Elastic Constant (anti-B}_{18}\text{)} = \begin{bmatrix} 20.49 & 0.55 & 7.42 & 0 & 0 & 0 \\ 0.55 & 23.12 & 2.17 & 0 & 0 & 0 \\ 7.42 & 2.17 & 18.61 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6.18 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12.08 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4.46 \end{bmatrix}$$

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