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SUPPLEMENTARY INFORMATION

Multi-faceted elastic flexibility of 1-naphthyl and 9-anthryl 2,2':6',2''-terpyridine crystals

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Table S1. Crystallographic data of **1** and **2**.

Compound	**1**	**2**
formula	$C_{25}H_{17}N_3$	$C_{29}H_{19}N_3$
formula weight	359.41	409.47
crystal system	orthorhombic	monoclinic
space group	*Pbca*	$P2_1/c$
a / Å	11.0002(6)	12.7668(17)
b / Å	9.8052(7)	14.4310(16)
c / Å	34.289(2)	11.6963(18)
α / º	90	90
β / º	90	104.463(12)
γ / º	90	90
V / Å^3	3698.4(4)	2086.6(5)
Z	8	4
T / K	300	293
R_1	0.0638	0.0841
R_1 (all data)	0.1125	0.2329
wR_2	0.1603	0.1953
wR_2 (all data)	0.1974	0.2924
G.O.F.	1.056	0.957
CCDC	2203397	2203398

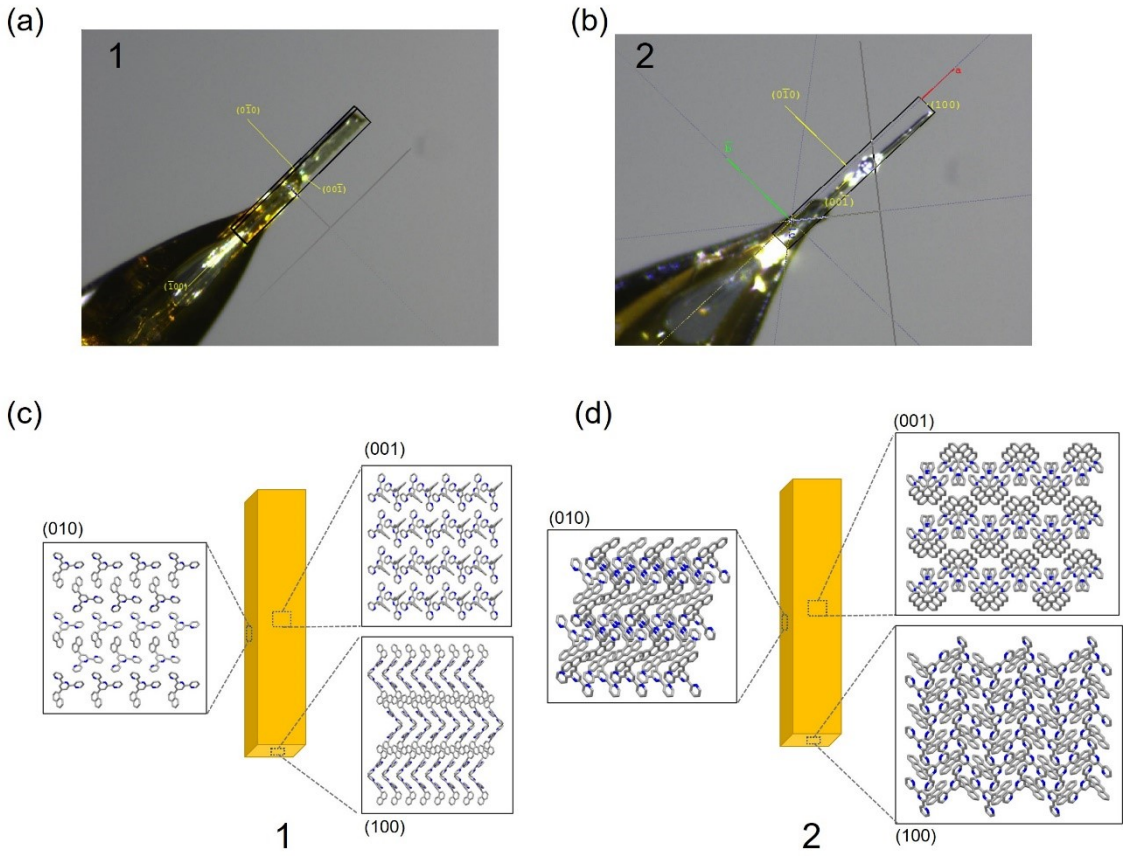

Fig. S1 The face indices for (a) **1** and (b) **2**, and respective schematic representation of the crystal with face indices (c, d).

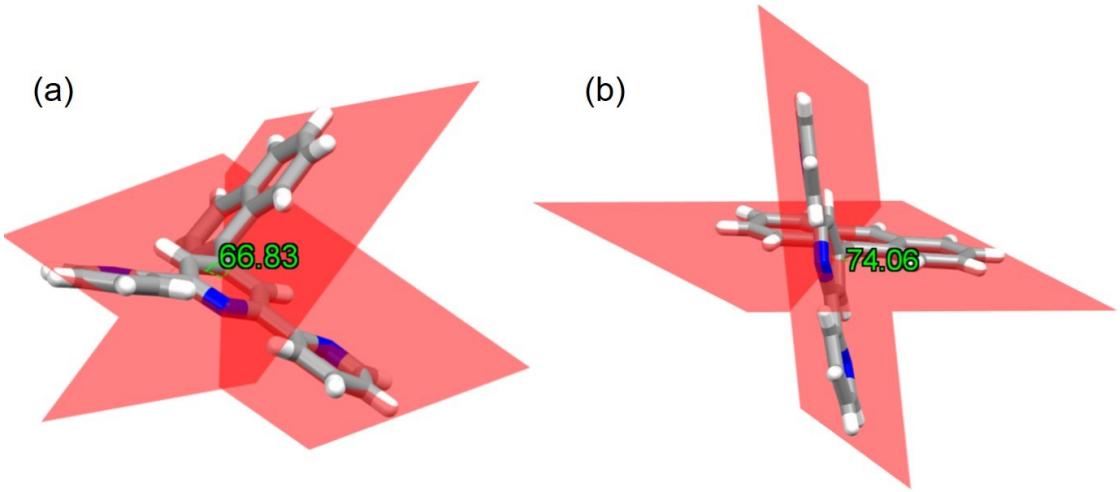

Fig. S2 Dihedral angles between the central pyridine ring of terpyridine and 4'-positioned substituents; **1** (a) and **2** (b).

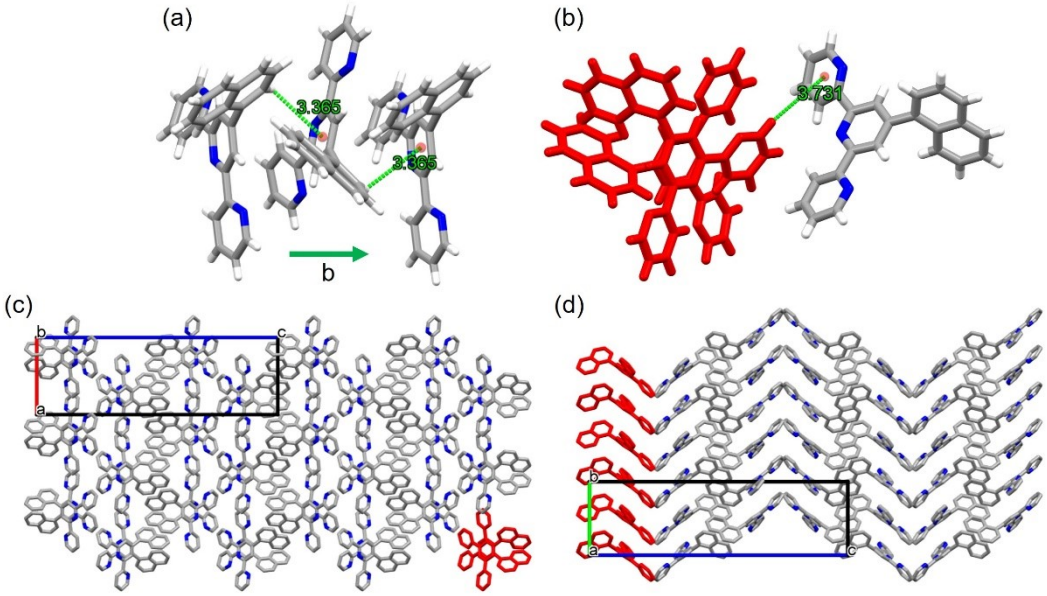

Fig. S3 Crystal structure of **1**. (a) One-dimensional chain via CH---π interactions (*d* = 3.365 Å) along *b*-axis. (b) CH---π interaction between 1D chain (*d*= 3.731 Å). Packing structures viewed down *b*- (c) and *a*-axis (d) (The molecules in 1D chain are red.).

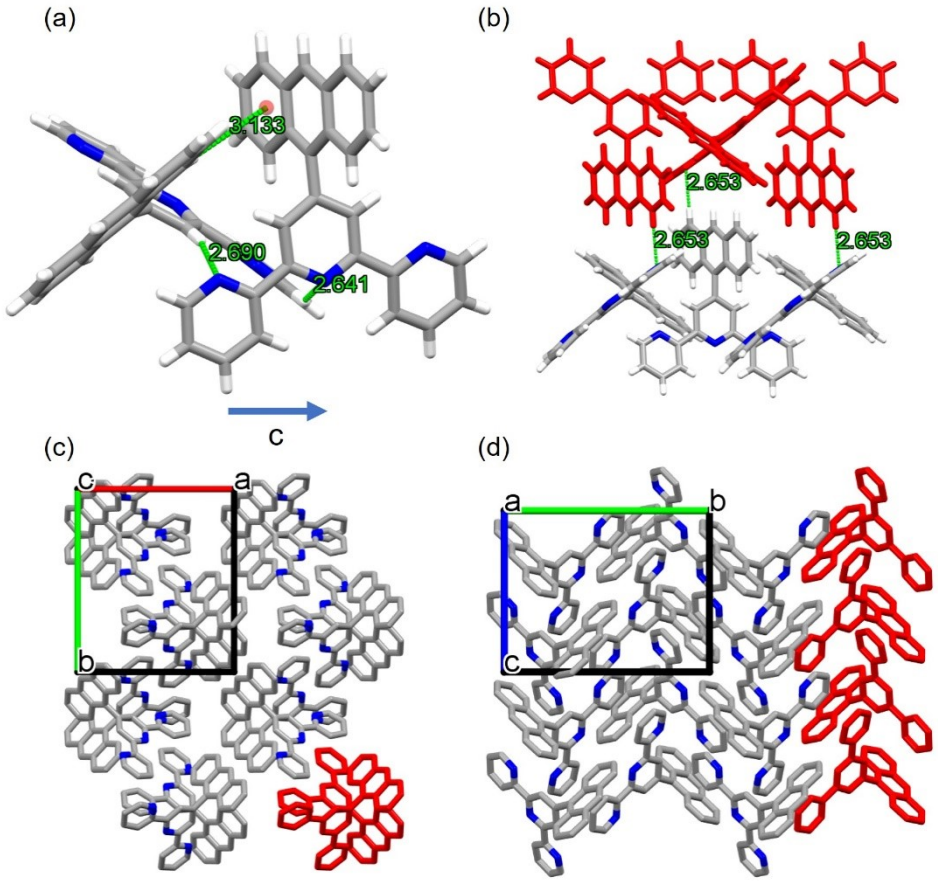

Fig. S4 Crystal structure of **2**. (a) One-dimensional chain via N---H interactions (*d* = 2.690 and 2.641 Å) and CH---π interactions (*d* = 3.133 Å) along *c*-axis. (b) Interactions between 1D chains via N---H (*d* = 2.653 Å). Packing structures viewed down *c*- (c) and *a*-axis (d) (The molecules in 1D chain are red.).

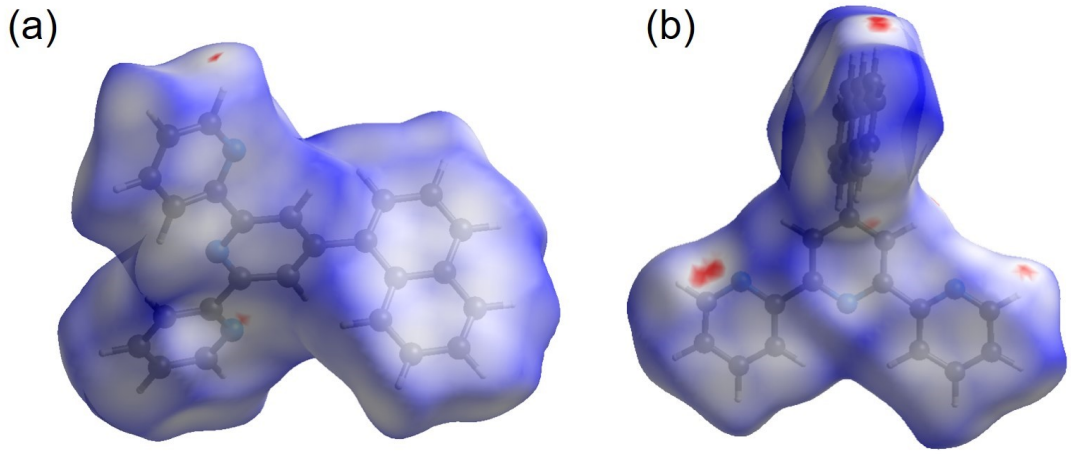

Fig. S5 Hirschfeld surface analyses of **1** (a) and **2** (b).

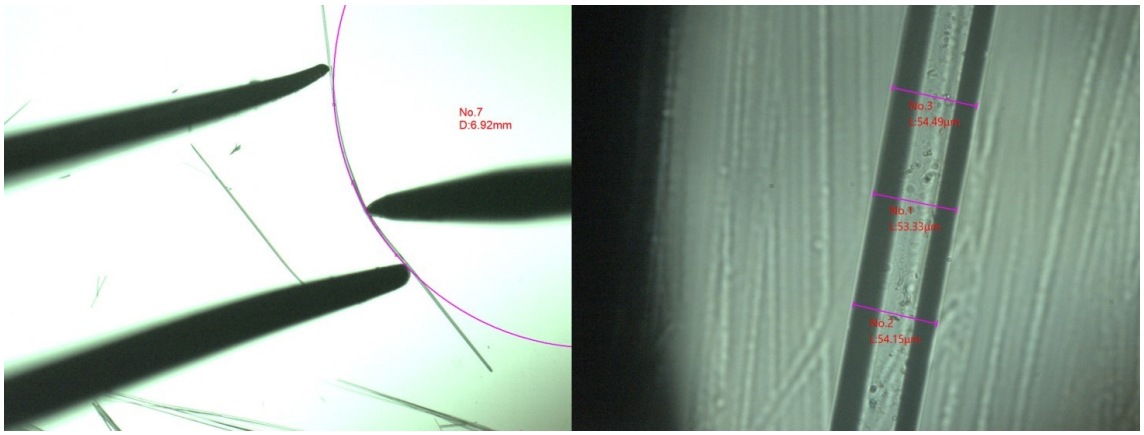

Fig. S6 Strain measurement for crystal **1** by applying force to (010). The thickness of crystal (right) and the radius of the curvature before cleavage (left).

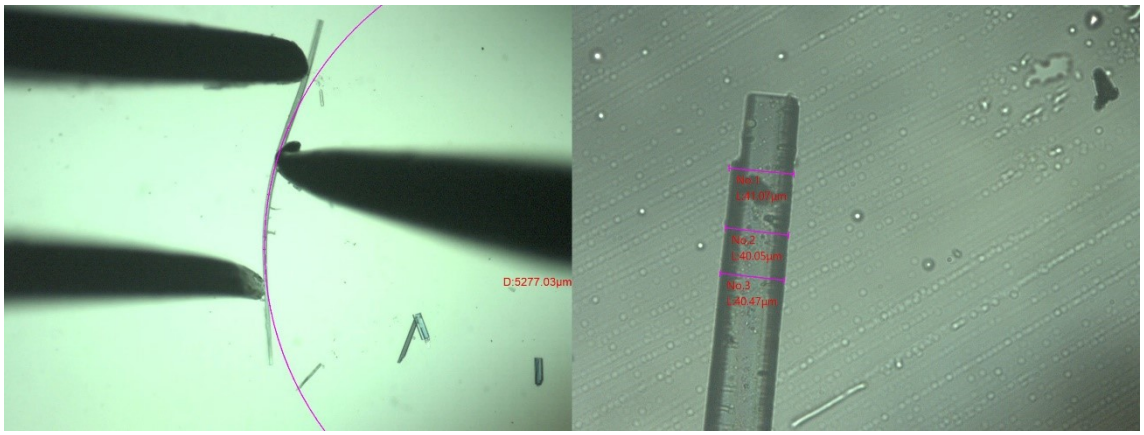

Fig. S7 Strain measurement for crystal **1** by applying force to (001). The thickness of crystal (right) and the radius of the curvature before cleavage (left).

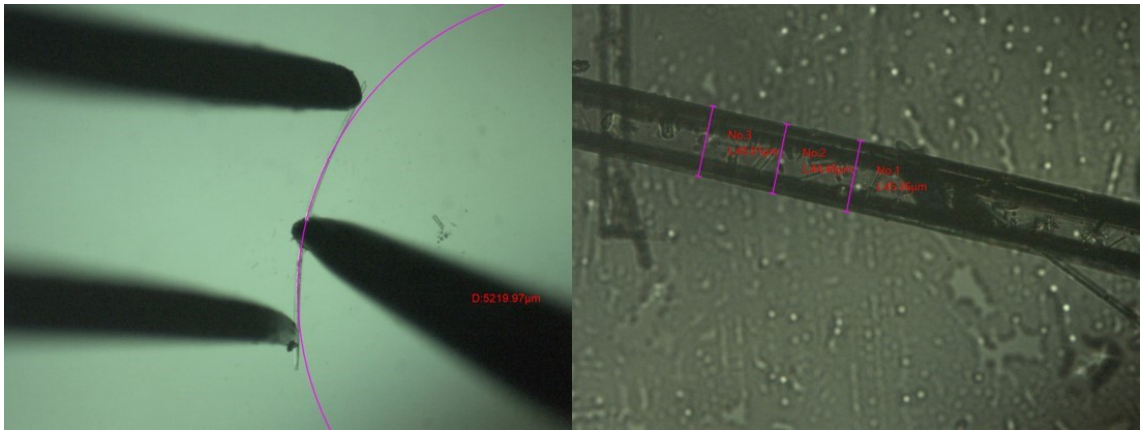

Fig. S8 Strain measurement for crystal **2** by applying force to (010). The thickness of crystal (right) and the radius of the curvature before cleavage (left).

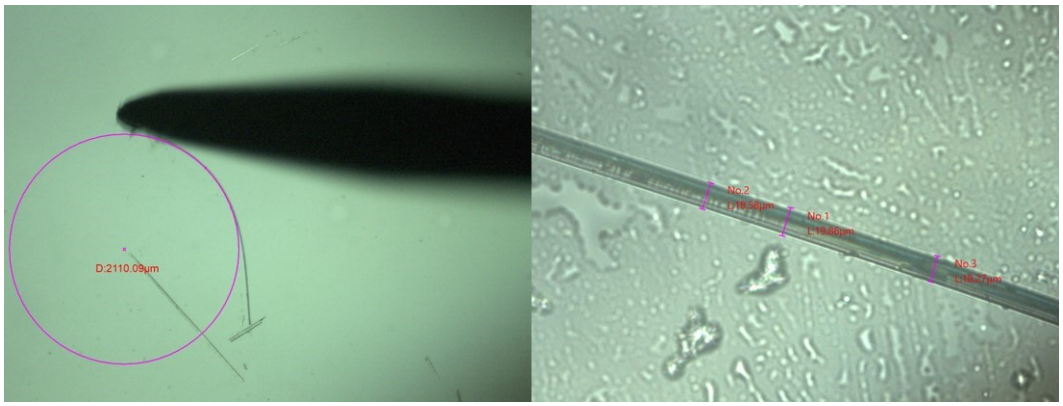

Fig. S9 Strain measurement for crystal **2** by applying force to (001). The thickness of crystal (right) and the radius of the curvature before cleavage (left).

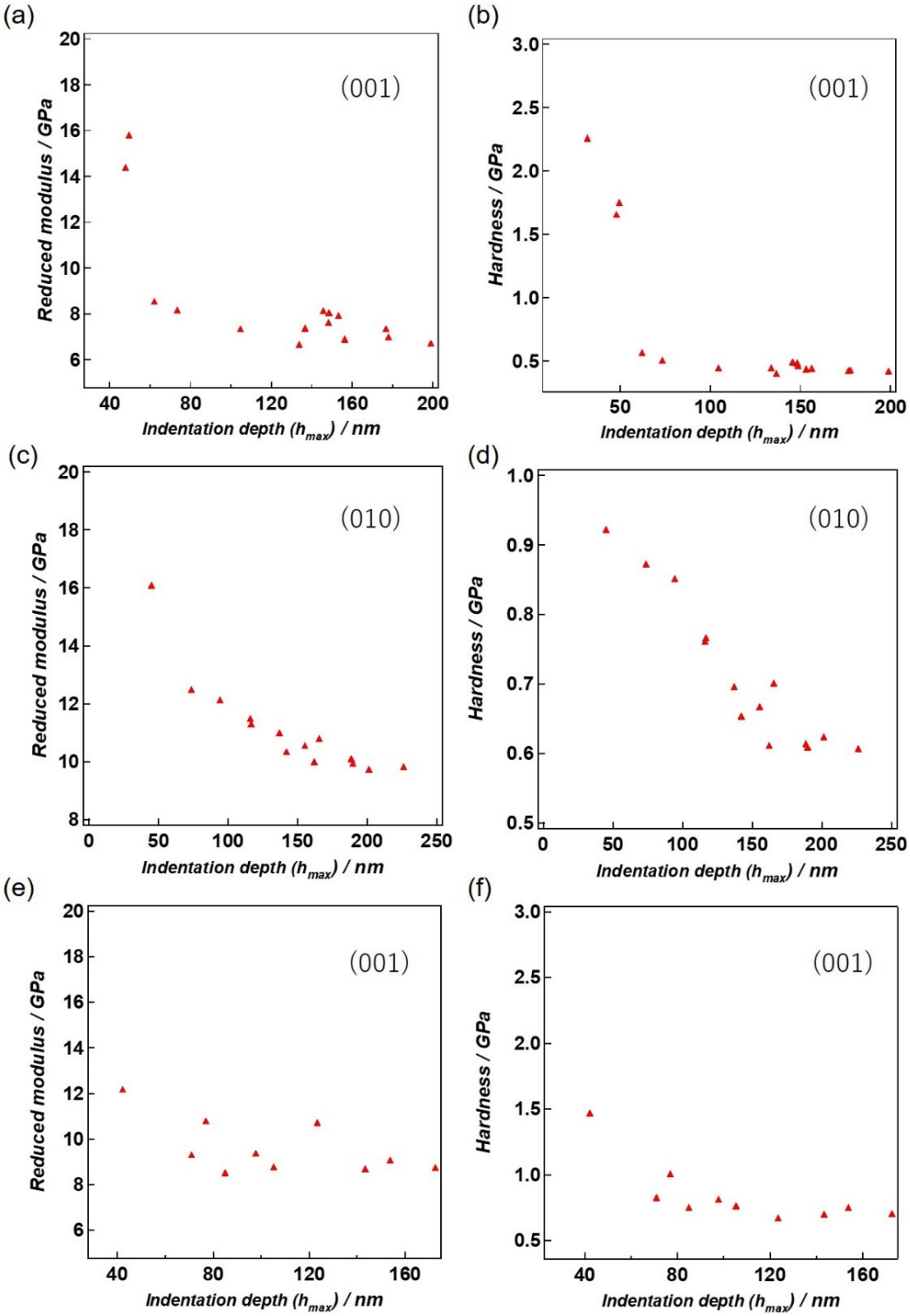

Fig. S10 Indentation depths (h_{max}) depending on 'Reduced modulus' (GPa) and 'Hardness' (GPa) on the surfaces of each crystal **1** (a-d) and **2** (e, f).

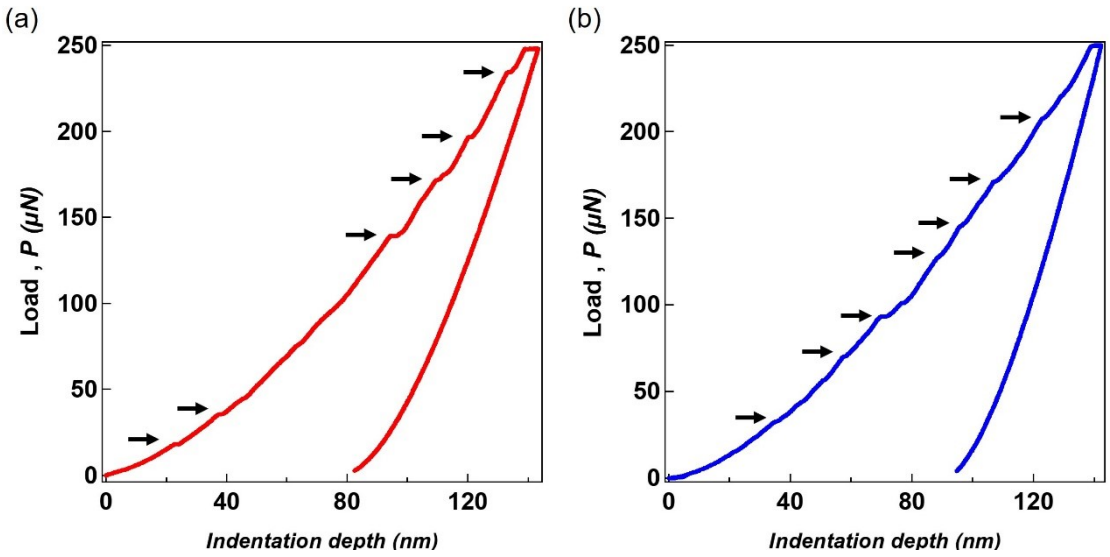

Fig. S11 *P*-h curves when the maximum load of 250 μN is applied on each crystal **1** (010) (a) and **2** (001) (b). Black arrows represent pop-ins.

Energy Framework Calculations

Energy frameworks for **1** and **2** were constructed from pairwise interamolecular interaction energy calculations (at crystal geometry) using the B3LYP/6-31G(d,p) molecular wave functions with CrystalExplorer17.5.[ref 20 in the main text] Total interaction energy decomposition into electrostatic, polarization, dispersion and exchange-repulsion terms can be obtained from a scaling scheme.

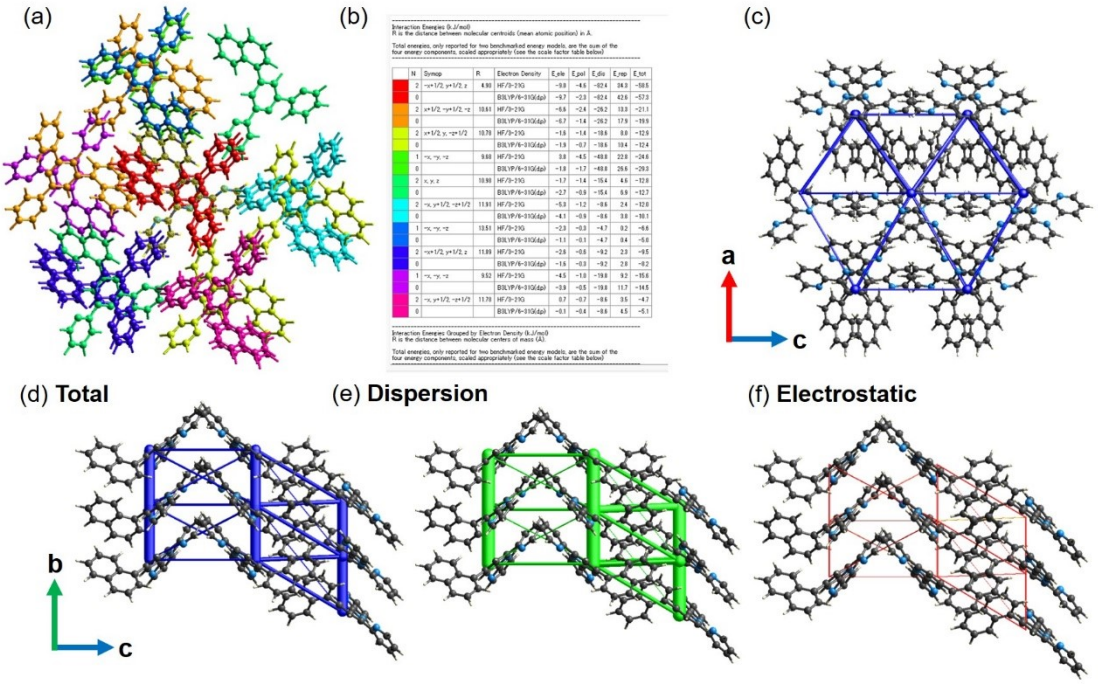

Fig. S12 (a, b) The interaction energies of various dimeric molecules estimated using CE-B3LYP method for **1**. (c) Energy frameworks in total interaction strengths viewed down the *b*-axis. Energy frameworks viewed down the *a*-axis are represented in Total (d), Dispersion (e), and Electrostatic energy (f).

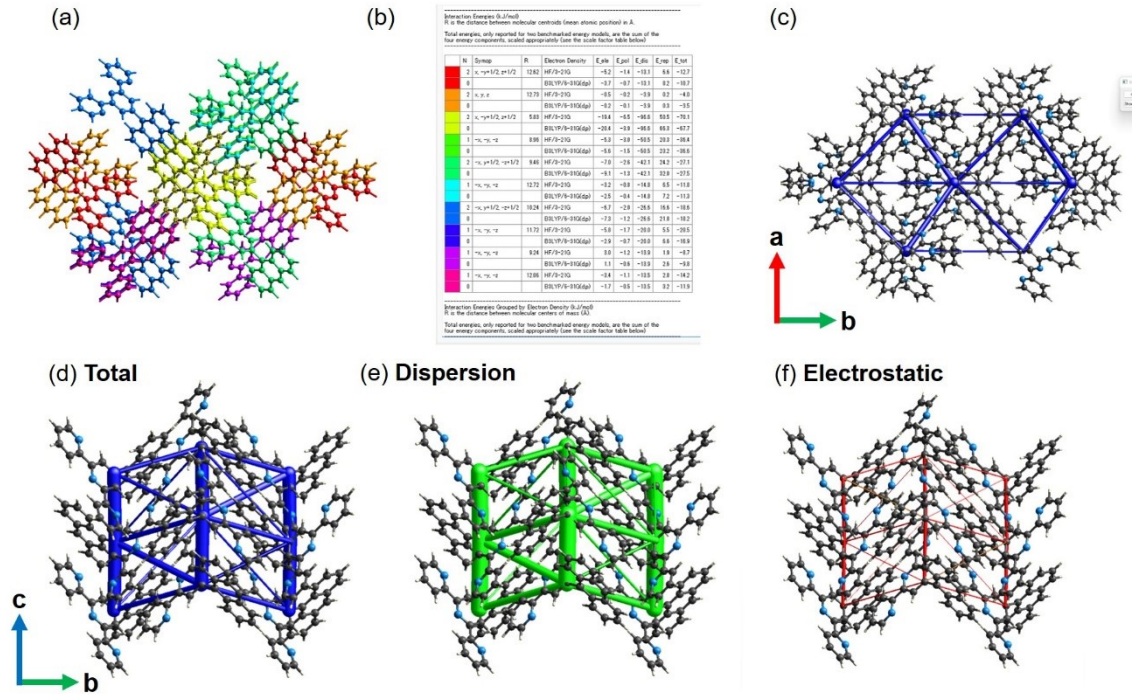

Fig. S13 (a, b) The interaction energies of various dimeric molecules estimated using CE-B3LYP method for **2**. (c) Energy frameworks in total interaction strengths viewed down the *c*-axis. Energy frameworks viewed down the *a*-axis are represented in Total (d), Dispersion (e), and Electrostatic energy (f).

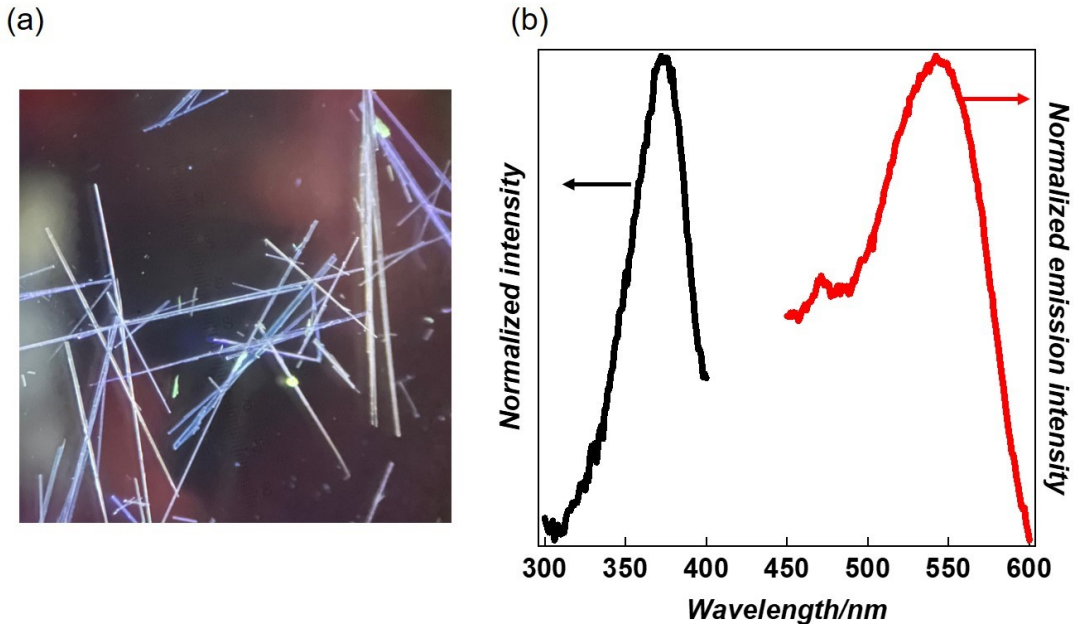

Fig. S14 (a) Photograph of crystals **1** under UV irradiation (365 nm). (b) Luminescence (λ_{ex} = 350 nm, red line) and excitation spectrum (λ_{mon} = 525 nm, black line) of **1**.

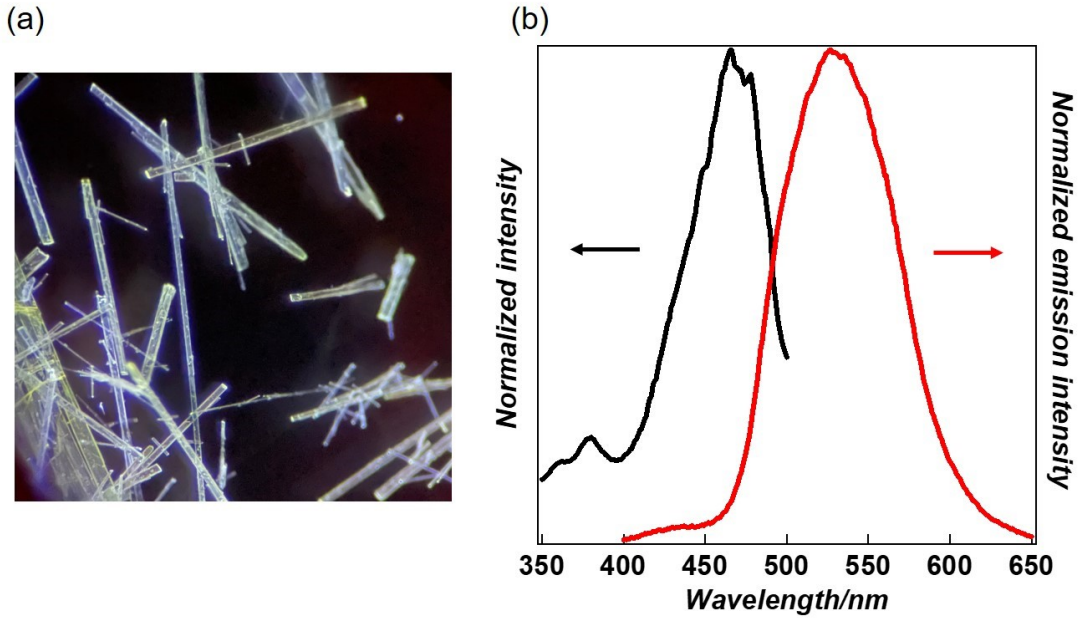

Fig. S15 (a) Photograph of crystals **2** under UV irradiation (365 nm). (b) Luminescent (λ_{ex} = 400 nm, red line) and excitation spectrum (λ_{mon} = 540 nm, black line).