Elastic organic semiconducting single crystals for durable all-flexible

field-effect transistors: insights into the bending mechanism

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1. Instrumental methods

Single crystal X-ray diffraction (SCXRD): SCXRD data was collected at 293 K for the crystal of DPP-diEt on a SuperNova, Eos diffractometer using monochromatic Cu-K α radiation having a 300 μ m beam size. The structure was solved by Olex2, (1.2.9 version) with the SHELXT structure solution program via intrinsic phasing algorithm and the ShelXL refinement package using Least Squares minimization was utilized to refine the structure¹⁻². Displacement parameters of all non-hydrogen atoms were refined anisotropically. Mercury (3.10.1 version) software was used to prepare all the crystal packing diagrams.

Powder X-ray diffraction (PXRD): The PXRD pattern was collected on a Rigaku Mini Flex with a Cu K α radiation (1.540 Å). The tube voltage and amperage were set at 40 kV and 15 mA, respectively. The instrument was previously calibrated using a silicon standard.

¹H-NMR and ¹³C-NMR: NMR analysis of DPP-diMe and DPP-diEt was performed on a JEOL 400 MHz NMR in CDCl₃ at 25 °C.

Nanoindentation: Crystals were mounted using Fevi kwik glue on a stainless-steel disk-shaped sample holder having a smooth surface in such an orientation so that the major faces would be indented. Face indices were identified from SCXRD and found that (011) is the major face of both compounds, DPP-diMe and DPP-diEt.

The experiments were carried out using a nanoindenter (Hysitron Triboindenter, TI Premier, Minneapolis, USA) with a three-sided pyramidal Berkovich diamond indenter tip of radius 150 nm having an in-situ Scanning Probe Microscopy (SPM) facility. Before nanoindentation, the tip area function was calculated from a series of indentations on a standard fused quartz sample. The indentations were performed under the load control mode fixing the maximum load constant (P_{max}) at 6 mN. The rates of loading and unloading were both 600 μ N/s with 5 sec duration and a 2 sec holding period was applied at the maximum indentation depth. SPM images of the indentation impressions were captured immediately just after unloading to avoid any time dependent elastic shape recovery of the residual impressions. The obtained P-h curves were analysed using the standard Oliver–Pharr method to extract the required parameters, elastic modulus (*E*), and hardness (*H*) of the crystals³.

2. Experimental procedures and theoretical calculations details:

Synthesis of diketopyrrolopyrrole (DPP) derivatives:

All the chemicals and solvents reported in this study were purchased and used as received. DPP derivatives were synthesised according to the literature procedure⁴.

For DPP-diMe: ¹H NMR (CDCl₃, 400MHz): 8.86 (d, J = 3.7 Hz, 2H), 7.62 (d, J = 4.4 Hz, 2H), 7.27 (dd, 2H), 3.59 (s, 6H).

For DPP-diEt: ¹H NMR (CDCl₃, 400MHz): 8.88-8.86 (m, 2H), 7.63 (dd, 2H), 7.28 (dd, 2H), 4.15 (q, J = 7.1 Hz, 4H), 1.36 (t, J = 7.1 Hz, 6H).

Energy frameworks calculations: The calculations pertaining to pairwise intermolecular interactions were performed using the software suite *CrystalExplorer*17.5 based on Gaussian *B3LYP-D2/6-31G (d, p)* molecular wave functions calculated using CIF files (obtained from SCXRD and DFT optimization)⁵.

Please note that the CIF obtained from experimental (SCXRD) and from periodic dispersion-corrected density functional theory (DFT) method are not identical. Hence, there are minute changes in the pairwise interaction energy values obtained from CIF (SCXRD) and from CIF (optimized at 0% strain), but the values from the two methods are comparable.

DFT strain-energy calculations: Before calculating the strain-energy curves for DPP-diMe and DPPdiEt, the equilibrium structure for each crystal was estimated using a periodic dispersion-corrected density functional theory method as implemented in VASP⁶⁻⁸, which uses the projector-augmented wave (PAW)⁹ method with plane-wave basis sets and PAW pseudo potentials. In all calculations, the PBE¹⁰ generalized gradient approximation (GGA) was used for the exchange-correlational functional coupled with the D3 dispersion-correction with Becke-Johnson damping¹¹. VASP input files were generated using the CIF2Cell¹² program. In all cases, a ^Γ-centered Monkhorst-Pack scheme was used to generate a tight K-point mesh with maximum K-point distance set to $2\pi \times 0.032$ Å⁻¹. In all calculations, the cut-off energy for the planewave basis set was set at 1000 eV. Within each selfconsistent field cycle, the convergence threshold was set at 1×10^{-5} eV and the geometry were considered converged when all forces were below 0.03 eV Å⁻¹. A two-stage geometry optimization protocol was adopted in calculating the equilibrium structure for each crystal. Initially, lattice parameters were fixed and only the atomic positions were optimized. This was followed by the simultaneous optimization of the lattice parameters and atomic positions, leading to the stress-free equilibrium crystal structure of DPP-diMe and DPP-diEt. Strain-energy curves were derived by applying uniaxial tensile or compressive strain to the needle axis of the equilibrium crystal structure in increments of 1%. Given that most mechanically compliant molecular crystals can only tolerate strains

of up to +/- 3%, a maximum of 3% tensile strain and -3% compressive strain was applied to each crystal. Upon the application of the strain, the crystal structure was subjected to fixed-cell geometry optimization in VASP using the same energy cut-off for the plane-wave basis set and convergence thresholds specified above. The strain energy (E_s) was estimated as the difference in the energy of the strained crystal at a particular strain value and the energy of the most stable crystal during the strain-energy simulations. Fixed-cell geometry optimizations at different strains were used to derive the strain-energy curves for two reasons. Firstly, microfocus synchrotron X-ray diffraction experiments on elastically bendable crystals has previously shown that the total volume of the crystals remains unchanged during elastic bending.¹³ Secondly, it is clear from the work of Yang *et al* which used a similar DFT model to that used here, that the strain-energy curves for strained crystals should be derived during structure relaxations at fixed-cell geometries¹⁴. Energy Frameworks calculations were used to estimate the percentage energy contributions of the dominant intermolecular interactions (see Table S1) in the equilibrium and strained crystals using *CrystalExplorer*17.5 ⁵ as per the settings outlined in the preceding section.

Molecular electrostatic potentials (MEPs): The molecular structure of DPP-diMe or DPP-diEt was extracted from the experimental crystal structure and subjected to gas-phase geometry optimization at the B3LYP/6-31G (d, p) level of theory using *GAUSSIAN09*¹⁵. The molecular electrostatic potentials (MEPs) for DPP-diMe and DPP-diEt were calculated by performing a single-point energy calculation at the same level of theory using the optimized molecular conformation as input. The resulting MEP was visualized in GaussView 5.0. Local minima and maxima on the MEP surface (0.0004 au isodensity surface) were calculated using a positive point charge in vacuum as a probe. The calculations lead to the interaction energy (in kJ mol⁻¹) between the positive point probe and the surface of the molecule at the point of contact.

Field effect transistor fabrication and measurement:

Bottom-contact top-gate field-effect transistors were fabricated on Cr/Au (3 nm: 22 nm), electrodes which were evaporated and patterned photo-lithographically onto precleaned PET substrates. This was followed by the solution-based casting of DPP-diMe and DPP-diEt to allow the growth of crystals. For that, 10 mg of pure DPP-diMe was added in 1 ml of (1:1) dry dichloromethane and toluene solvent mixture and after complete dissolution, the solution was placed in glove box and drop casted on substrate and left it for 15 mins. Same dropcasting procedure was followed for DPP-diEt, although here toluene solvent was used instead of dichloromethane toluene mixture and little heat was applied to dissolve all the compounds to make 10 mg/ ml solution. Cytop dielectric layer was then spin-coated over the films and annealed at 90 °C for 20 min. The devices were then completed by evaporating the

Au gate electrode (60 nm) through a shadow mask. FET characterization was performed using an Agilent 4155B parameter analyzer. The performance parameters of the devices were extracted in the saturation regime from the transfer characteristics curves by using the equation: $I_{ds} = (\mu_{FET}WC/2L) (V_g - V_{th})^2$, where I_{ds} is the drain current, W and L are, respectively, the channel width and length, C is the capacitance per unit area of the gate insulator layer, and V_g and V_{th} are the gate voltage and the threshold voltage, respectively. The mobility values reported are the median value obtained from the measurements performed on three devices in each case which are representative of the general trends in these molecular crystals. For applying strain on the flexible FETs, the devices were wound around metallic rods of specific radius (5 mm, 10 mm and 20 mm) for 5 minutes and then transfer characteristics were measured after releasing the strain.

Result and discussion:

Crystal growth: DPP-diMe crystals were grown in 5-7 days from 1:1 dichloromethane and toluene solution whereas DPP-diEt crystals were grown from toluene solution within 5-7 days by using slow evaporation method. Single crystal structure of DPP-diMe was reported in literature⁴ (REF Code: OVOVUS with deposition number 1505240) in a study related to singlet fission (SF) in polycrystalline thin films. Single crystal structure refinement parameters of DPP-diEt are provided in Section 12 below. We have run the pre-experiment analysis in case of DPP-diMe to match the cell and index the faces.

Calculation of maximum bending strain in the DPP-diMe crystals and face indexing images of original DPP-diMe and DPP-diEt crystals.



Figure. S1. a) Calculation of maximum strain that DPP-diMe crystals can withhold (prior to the onset of fracture). b) and c) Face indexing images of pristine DPP-diMe and DPP-diEt crystals, respectively.

The elongation or contraction ratio compared to the original crystal is calculated as follows:

For a crystal of thickness *d*, radius of curvature r (Figure. S1a)

Strain (
$$\varepsilon$$
) = d/2r

Several crystals of DPP-diMe with comparable morphologies ($d = 50 - 75 \mu m$) were subjected to elastic bending tests (qualitative) while simultaneously recording the videos using a high-speed camera attached to a microscope. The video grabs of frames, just prior to fracture point (Figure. S1a), were used to calculate

the maximum bending strain (ε) of the crystal. The ε of the DPP-diMe crystal was calculated to be in the range of 3 – 6 %. Since the DPP-diEt crystals fractured without any appreciable bending deflection, we could not quantify their strain limit (and assumed it to be a negligible quantity).

(a) (b) (c) (68,8) (c) (68,

3. Energy frameworks calculations of DPP-diMe and DPP-diEt:⁵

Figure. S2: Total interaction energy frameworks for the DPP-diMe. Tube size 100 and energy cut-off 5 kJ/mol.



Figure. S3: Molecular structure pairs and the interaction energies (kJ/mol) obtained from energy frameworks calculation for DPP-diMe. Scale factors are in the lower table. The error value in interaction energy is ± 1 kJ/mol.



Figure. S4: Total interaction energy frameworks for the DPP-diEt. Tube size 100 and energy cut-off 5 kJ/mol.



Figure. S5: Molecular structure pairs and the interaction energies (kJ/mol) obtained from energy frameworks calculation for DPP-diEt. Scale factors are in the lower table. The error in interaction energy value is ± 1 kJ/mol.

4. DFT strain-energy calculations:

Table S1: Energy frameworks contributions of specified interactions as a function of the applied uniaxial (a-axis) strain

	DPP-diMe		DPP-diEt	
Applied Uniaxial (<i>a</i> -axis) Strain	π stacking energy (kJ/mol)	C-H…O (kJ/mol)	π stacking energy (kJ/mol)	C-H…O (kJ/mol)
+ 3 %	-65	-17	-61	-19
0 %	-68	-17	-65	-20
- 3 %	-70	-17	-67	-20

5. Molecular electrostatic potentials (MEPs)



Figure. S6: Molecular electrostatic potentials for (a) DPP-diMe and (b) DPP-diEt. The potential on the C=O group of both compounds is indicated.

6. Histogram plots of DPP derivatives evaluated from performed Nanoindentation measurements:



Figure. S7: Young's modulus (a) and hardness (b) obtained from a total of 20 indents performed on four different samples of DPP-diMe. Results are presented as histograms.



Figure. S8: Young's modulus (a) and hardness (b) obtained from a total of 20 indents performed on four different samples of DPP-diEt. Results are presented as histograms.

7. FET characterization in absence and on electrostatically bonded organic crystals with Au S-D:

In order to ensure that the charge transport properties originate from the DPP-semiconductor, we have performed measurement without the crystals and also when the crystals are electrostatically introduced on the lithographically patterned Au S-D electrodes (Figure. S9). However, we did not observe any gate modulation and the observed current values of 1-100 *p*A for Vg = -60 V, V_d = -60 V on these devices. From these measurements it is adequately clear that the observed changes in the transport properties upon bending originated from the DPP-crystals and the variation in the transport properties upon straining is majorly attributed to the semiconductor and not any other external factors.



Figure. S9: a) Typical transfer characteristics measured on a DPP-diMe crystal when electrostatically introduced on Si/SiO_2 with lithographically patterned Au S-D electrodes. b) transfer characteristics measured on a Si/SiO_2 substrates with lithographically patterned Au S-D electrodes in absence of semiconducting DPP based crystals.

8. Crystal growth on flexible FETs: Devices prepared with solution grown crystals exhibit a typical needle-like characteristics which is shown in the SEM image, Figure.S10.



Figure. S10: Typical SEM image of (a) DPP-diMe and (b) DPP-diEt crystals grown on top of the lithographically patterned flexible devices.

9. Powder X-ray diffraction:

In order to ensure that the crystals obtained from solution processed deposition on top of the flexible substrate is of similar quality in terms of crystallinity, we performed PXRD measurements on these flexible substrates with solution grown crystals. The PXRD pattern for both the organic crystals, DPP-diMe and DPP-diEt, were compared with the simulated PXRD pattern obtained from the corresponding SCXRD analysis and a clear correlation between the peaks is observed as shown in Figure. S11.



Figure. S11. Powder x-ray diffraction patterns of DPP-diMe and DPP-diEt compounds after drop casting on PET substrates along with their simulated PXRD patterns.

10. Percolation analysis of the charge transport in flexible organic crystal-based FETs:

To optimize the FET fabrication, devices were fabricated from different concentration of DPP-diMe solutions. It was observed that the channel current increases with increase in concentration of the solution. Interestingly, upon increasing the solution concentration, we observed an enhancement in the channel current and decrease in the hysterics characteristics (Figure. S12).



Figure. S12: Typical transfer characteristics measured on flexible FETs fabricated with DPP-diMe solutions of concentration a) 2 mg/mL, b) 5 mg/mL, and c) 10 mg/mL.

Optical and SEM imaging of the channel area was performed on the devices. It was observed that with increasing the concentration of the solution used for preparing the crystals, the coverage of the organic crystals on the channel area increased (Figure. S13), majorly due to the increment in the nucleation sites.



Figure. S13: Typical optical microscopy images of the channel area for the devices fabricated with (a) 2 mg/ml, (b) 5 mg/ml of DPP-diMe. Corresponding SEM images of the channel area depicting the variation in crystal density for devices fabricated with c) 2 mg/mL, d) 5 mg/mL DPP-diMe solution. Scale bar is 20 μ m.

Based on the optical and microscopic images it can be ascertained that this enhancement in the device performance can be majorly attributed to an improvement in percolation pathways resulting from higher density of the crystals. In a typical 2D percolation network, the relationship between the percolation threshold (N_c) and tube length (L) takes the form, L (π N_c)^{1/2} = 4.2. Applying this condition for the present case where the crystals have an average length ~ 10 µm, a percolation threshold of ~ 0.05 µm⁻² is obtained. Although devices fabricated with a 2 mg/mL solution concetration have a crystal density > 0.05 µm⁻² due to the low coverage over the flexible substrate, it is expected that the gate bias potential V_g does not get

completely translated into interface charges. Consequently, the trap density estimated from the transfer characteristics is observed to decrease from 10^{13} cm⁻²eV⁻¹ to 10^{12} cm⁻²eV⁻¹ as the effective channel coverage increases from ~ 5 % to around ~ 90 %. Hence, in order to obtain a close estimate of the intrinisic transport properties of the materials and correlate it to the mechanical durability of the material we ensured that both DPP-diMe and DPP-diEt were fabricated with the condition which corresponds to at least a ~ 90 % coverage of the channel area. Typical optimized output and transfer characteristics of flexible FETs fabricated from DPP-diMe and DPP-diEt is shown in Figure. 6b,c,f,g.

To test the mechanical durability of the devices, crystals were exposed to strain by winding them around metallic rods of specific radius (5 mm, 10 mm and 20 mm) for 5 minutes and then transfer characteristics were measured after releasing the strain.



Figure. S14: Transfer characteristics measured on a bottom contact top gate flexible device (L = 20 μ m, W = 1 mm) with different bent radius for (a) DPP-diMe and (b) DPP-diEt based crystals. (c) Variation in the μ_{FET} of the flexible devices fabricated with DPP-diMe crystals (black) and DPP-diEt (blue) when bent at different radii. Error bars are indicative of the mean deviation of measurement over 3 devices for the figure. (c).

11. Statistical distribution of mobility:

Statistical distribution of mobility measured on 16 devices indicating the robustness of the mobility estimation is presented below.



Figure S15: Statistical distribution of field effect mobility measured on different devices fabricated with DPP-diMe and DPP-diEt semiconductors exhibiting the general reliability of the measurements. Each point corresponds to one FET device taken for mobility measurement.

12. Evaluation of effect of contact resistance:

In order to understand the effect of contact resistance on the FET characteristics, we estimate the resistance from the linear regime of the output characteristics and obtain the contact resistance through the transfer line method. The contact resistance is observed to be at least one to two orders of magnitude higher than the channel resistance indicating that the transport is not contact limited in these devices.



Figure S16: Transfer line measurements performed on FETs fabricated with DPP-diMe crystals and brittle DPP-diEt self-assembled crystals.

13. Mobility variation with strain cycles in flexible organic crystal-based FETs:

To obtain the number of cycles the flexible FETs fabricated from DPP-diMe can be operated reliably, we extrapolated the plot till the $\mu_{\text{FET}} \sim 10^{-5} \text{ cm}^2/\text{Vs}$. From Figure. S15 it can be observed that flexible FETs fabricated from DPP-diMe can be operative till 275 cycles of straining while bent at 5 mm radius.



Figure. S17: Variation of μ_{FET} upon multiple cycle of straining at a bend radius of 5 mm for the DPP-diMe extrapolated till μ_{FET} drops to 10⁻⁵ cm²/Vs.

14. Crystallographic Information: Crystallographic Table with structural refinement parameters of DPP-diEt.

Temperature (K)	293 K		
Formula	$C_{18}H_{16}N_2O_2S_2$		
Formula Weight	356.45		
Crystal System	monoclinic		
Space group	$P2_1/n$		
a/ Å	5.3077(2)		
b/Å	10.6410(3)		
c/Å	14.3047(4)		
α/°	90		
β/°	97.421(3)		
γ/°	90		
V/ Å ³	801.151		
Ζ	2		
$D_{\rm c}/{\rm g~cm^{-3}}$	1.478		
μ/mm^{-1}	3.126		
F(000)	372.0		
θ range/°	5.196-65.783		
Reflections collected	6826		
Unique reflections	1391		
reflections $I > 2\sigma(I)$	1309		
R _{int}	0.0467		
Goodness of fit (F^2)	1.081		
$R1 (I > 2\sigma(I))$	0.0510		
$wR2(I > 2\sigma(I))$	0.1487		
CCDC No.	2102226		

15. Supplementary movies:

The supplementary movies S1 and S2 were recorded via Leica microscope.

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