Electronic Supplementary Information (ESI) for:

Micrometer long oriented one-dimensional wires and two-dimensional sheets from a bis-urea functionalized dialkoxy-naphthalene organogelator

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Experimental Section:

Surface Potential measurements:

We have prepared 0.5 mg/ml stock solution of **DAN-U** solution in chloroform. We have spread 80 µl from the stock solution at the air-water interface of milli-Q water (resistivity 18.2 MΩ cm) and air. A waiting time for 10 minutes was allowed for solvent evaporation, thereafter the surface pressure (**π**)-area (A) isothem and suface potential (ΔV)-area (A) isotherm were measured. Surface potential at the air-water interface was measured by Trek Electrometer 320 by using the following formula:[1,2]

$$\Delta V = \frac{\mu}{\varepsilon\varepsilon_0 A} \quad \text{.....(1)}$$

Where where μ is the effective molecular dipole moment perpendicular to the air-water interface, $\mathcal{E}$ is the permittivity of the monolayer, $\mathcal{E}_0$ is the permittivity in a vacuum, and A is the area per molecule. Eequation 1 reveals that surface potential is directly poportional to the effective molecular dipole moment which correlates the steep increase in surface potential with the incrase in effective molecular dipole moment at air-water interface.

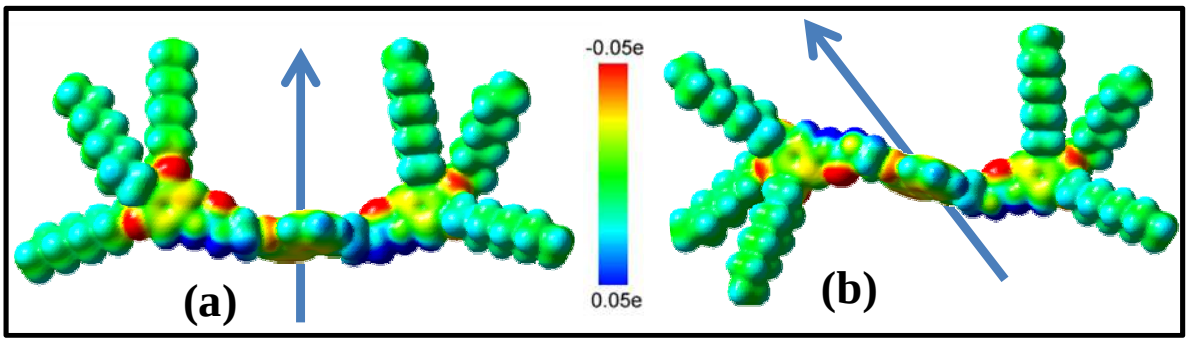

Figure S1 Possible conformaion of DAN-U molecule at air-water interface with dipole moment direction indicated by arrows. (a) Charge distribution for "cis" coformation (b) Charge distribution for "trans" conformation.

The structures of the *cis* and *trans* conformers were optimized using hybrid DFT (Density Functional Theory) functional B3LYP[3] using 6-31G** basis-sets for all atoms employing G09[4] software. The energy difference between the *cis* and the *trans* conformers is found to be small (~0.4 kcal at 300K) and we expect both conformation to co-exist under normal conditions. The end-to-end distances as measured from the optimized structures also are very similar (~44.5 Å). However, the overall height of the **DAN-U** is found to be more for the *trans* isomer (22 Å) in comparison to the *cis* isomer (17 Å). In the *cis* isomer, the urea groups appear in the same direction while in the *trans* isomer, they exist in opposite direction. The calculated dipole moment for the *cis* isomer is 5.64 D in comparison to 1.14 D for the *trans* isomer. The electronic charge density in the molecules are calculated using Mulliken's method.[5] Electrostatic potential (ESP) at a point in the space around a molecule gives an indication of the net electrostatic effect produced at that point by the total charge distribution of the molecule, which can be correlated with total dipole moments, partial charges and chemical reactivity of the molecules. It also provides a visual understanding of the relative polarity of the molecule. The different values of the electrostatic potential represented by different colors in the plots; red represents the regions of the most negative electrostatic potential, blue represents the regions of the most positive electrostatic potential and green represents the region of zero potential. Such mapped electrostatic potential surfaces have been plotted for the *cis* and *trans* conformers of **DAN-U** using Gauss view software. **DAN-U** remain flat with

cis conformation at air-water interface and the direction of the dipole monent is perpendicular to the air-water interface as shown in the figure S1a.

AFM Analysis:

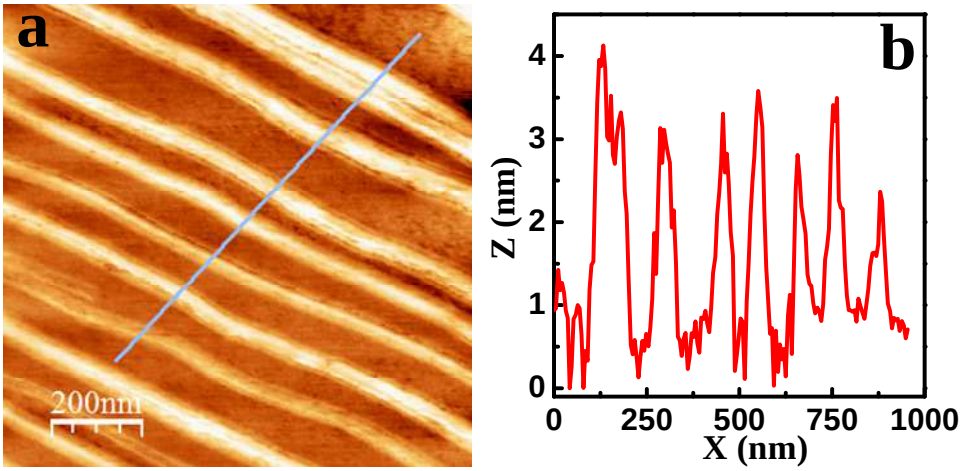

Figure S2 (a) AFM topography image of molecular wires formed by **DAN-U** π-systems. For AFM studies, freshly cleaved mica was used and film lifted at surface pressure 14mN/m. (b) Height profile line scan monitored on different molecular wires suggesting that the heights of these molecular wires are less than 4 nm.

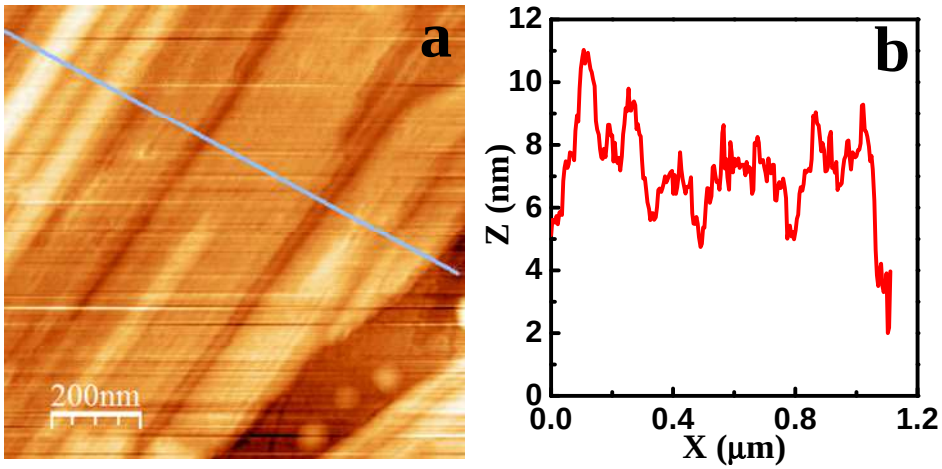

Figure S3 (a) AFM topography image lifted after collapse pressure on top of freshly cleaved mica shows formation of 2D molecular sheets. (b) Height profile line scans over one micrometer shows that heights of 2D molecular sheets is double in comparison to the molecular wires lifted at surface pressure 14mN/m (Figure S2) suggesting a bi-layer of **DAN-U** molecules within the sheets.

References:

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