SUPPORTING INFORMATION

KINKED ROW-INDUCED CHIRALITY DRIVEN BY MOLECULE-SUBSTRATE INTERACTIONS

Sergii Snegir,^{a,b} Yannick J. Dappe^c, Oleksiy L. Kapitanchuk^d, Delphine Coursault^e and Emmanuelle Lacaze^{*a}

- ^{a.} Sorbonne Université, Faculté des Sciences, CNRS, Institut des Nano-Sciences de Paris (INSP), 4 pl Jussieu 75005 PARIS, France.
- ^{b.} University of Konstanz, Konstanz, Germany.
- ^{c.} 3SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France
- d. Bogolyubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine
- e. Université de Bordeaux, CNRS, LOMA, UMR 5798, F-33400 Talence, France

Herringbone (22×\sqrt{3}) reconstruction of Au[111]:



Figure S0. STM image of freshly prepared Au[111] surface with the Au[111]/ $22 \times \sqrt{3}$ reconstruction pattern without adsorbed 10CBreconstruction pattern.



Figure S1. a) HOMO and LUMO of a single 10CB molecule. – b) The potential for a single phenyl rotation related to the torsion angle, ψ , shown in the inset (lowest energy structure assigned as being at 0 eV). The equilibrium ψ value is 37°, in agreement with previous results ^{30, 44} and the potential values appear small enough to allow for an easy rotation – c) the bending potential related to the angle φ (lowest energy structure assigned as being at 0 eV). In contrast with the potential values are larger allowing for not easy bending.

Using the experimental observations we built schematic simplified models of molecular packing on HOPG, MoS_2 and on Au(111), represented on Fig.S2, S4, S5.



Figure S2. Packing model of 10CB molecules on the HOPG surface according to STM results (only the fan-shape of the cyanobiphenyl structure is not shown, instead we colored the molecules in red/yellow color that undergo the strongest dislocation in real STM images (Fig.S3) due to the fan-shape structure within a unit cell). The specific site carbon atoms of the underlying HOPG surface is colored in dark gray.



Figure S3. STM images of 10CB on HOPG surface recorded with the same tip under It = 1.8 pA; Ut = $350 \text{ mV} - \mathbf{a}$) and It = 2 pA, Ut= 0.28 V b). Black and white arrows points on some molecules at the edges of a unit cell is higher than for other molecules. Changing the tip scanning direction with respect to the row direction allows improving the STM contrast of the molecules at the edges. However, the optimal STM bias, current and scanning orientation for visualization of the unit cell edges can vary from the one presented above due to the different shapes of the apexes of mechanically cut STM tips.



Figure S4. Packing model of 10CB molecules on the MoS_2 surface according to STM results (only the fan-shape of the cyanobiphenyl structure is not shown).



Figure S5. Model of 10CB molecular packing on Au[111] according to STM results (only the fan-shape of the cyanobiphenyl structure is not shown), with Au atoms shown in yellow. P (period of packing along the substrate crystallographic direction) and α (the angle between the average row orientation associated with the kinks and the substrate

crystallographic direction parallel to the short side of the cell) is shown. The red curved line follows the position of the $-CH_3$ terminal groups of the 10CB. The black stars show the distance between extremities of alkyl chains of neighbouring rows in the middle of the cell, whereas, within the red ellipses, it is shown at the proximity of the kinks.



Figure S6. The STM image of 10CB SAM on top of Au[111]/22× $\sqrt{3}$ reconstruction.



Figure S7. Van der Waals radius visualization of two cyanobiphenyl groups illustrating the overlapping that occurs for a distance 6Å.



DTF calculation of adsorbed cyanobiphenyl groups on Au(111):

Figure S8. Evolution of the cyanobiphenyl/Au(111) interaction as a function of the localization of Au(111).