Supporting Information

Fabrication of One Dimensional Zigzag [6,6]-Phenyl-C_{61}-Butyric Acid Methyl Ester Nanoribbons from Two Dimensional Nanosheets

Eduardo Gracia-Espino[1,2,‡], *Hamid Reza Barzegar* [1,3,‡], *Tiva Sharifi*[1], *Aiming Yan*[3], *Alex Zettl*[3] *and Thomas Wågberg*[1,*]

[1]Department of Physics, Umea University, 90187 Umea, Sweden

[2]Department of Chemistry, Umea University, 90187 Umea, Sweden

[3]Department of Physics, University of California, Berkeley, Lawrence Berkeley National Laboratory, Kavli Energy NanoSciences Institute at the University of California, Berkeley and the Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA

[‡] Both authors have contributed equally to this work.

Corresponding author, email: Thomas.Wagberg@physics.umu.se

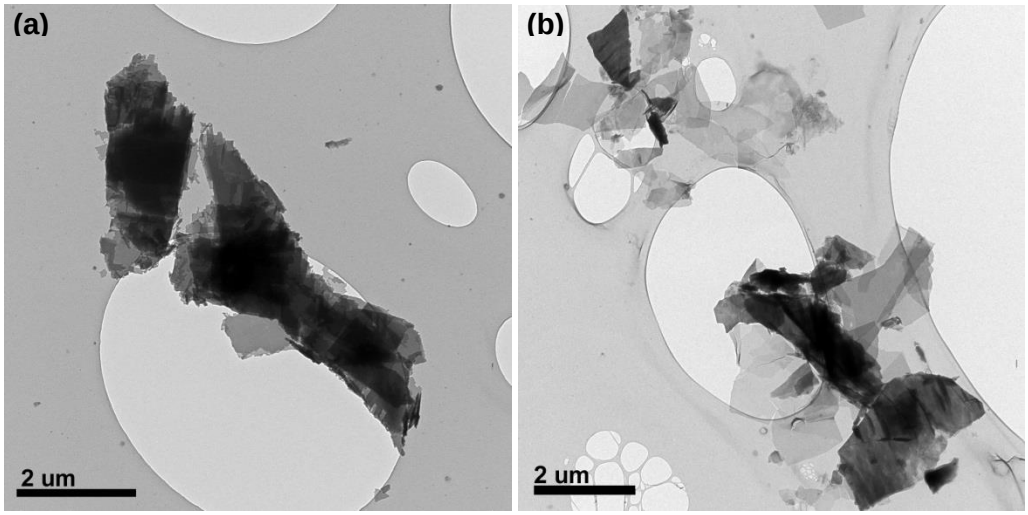

Figure S1. TEM micrographs of: (a) large PCBM crystal produced by static LLIP method, (b) PCBM crystals after sonication, showing that they can be exfoliated to thinner PCBM sheets.

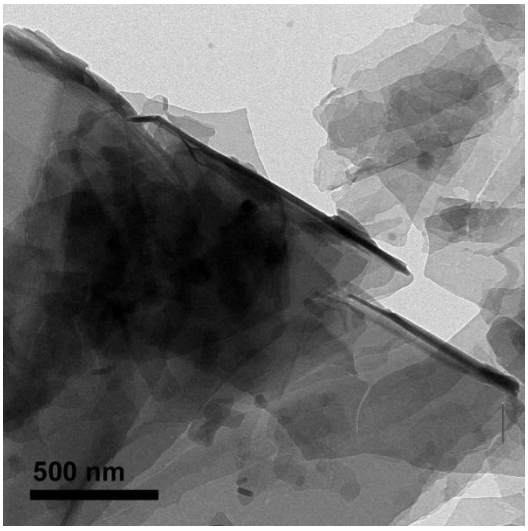

Figure S2. TEM image showing the initial folding step of the PCBM nanoribbon formation.

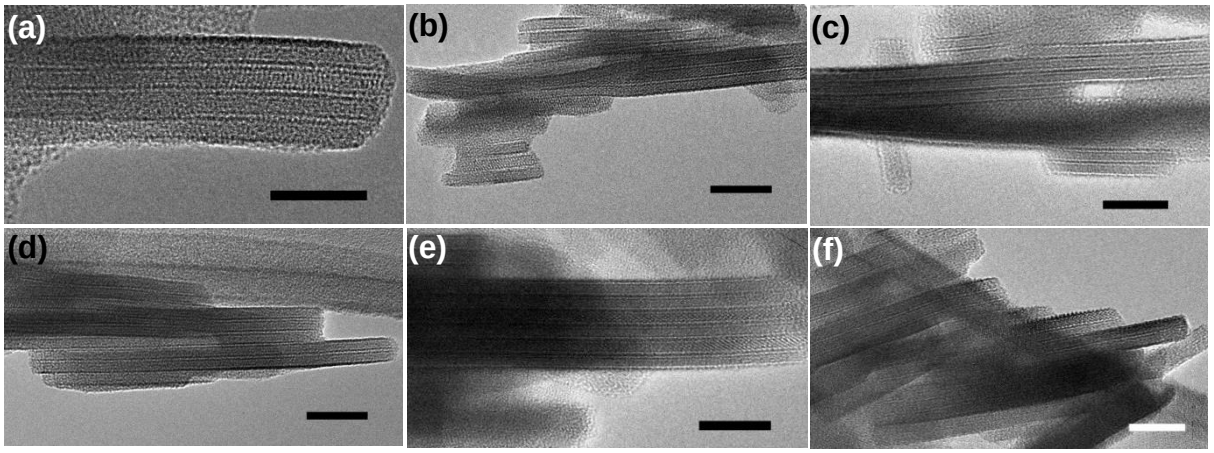

Figure S3. High resolution TEM images of PCBM nanorods revealing that each rod consists of several nanoribbons. Scale bar 20 nm.

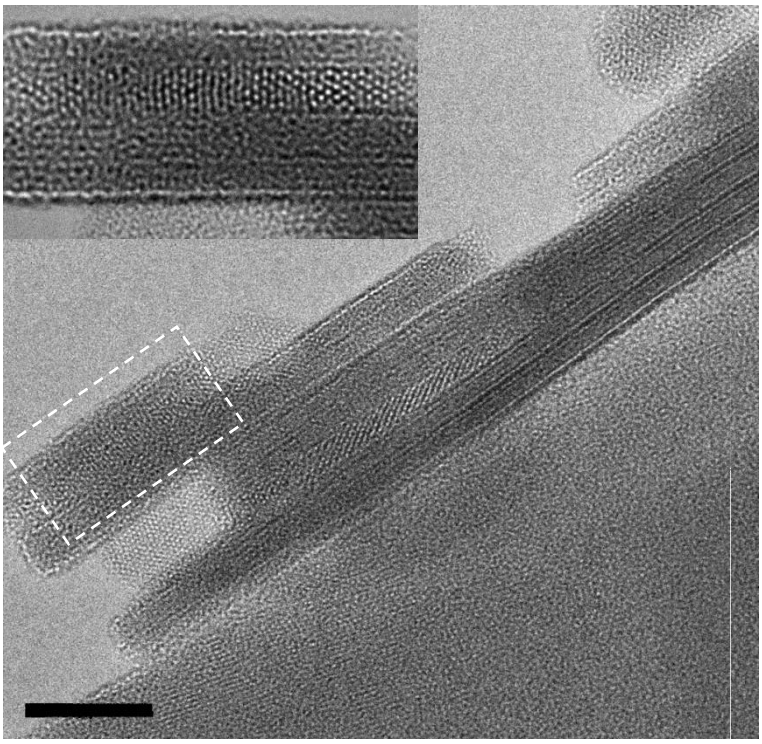

Figure S4. High resolution TEM image of PCBM nanorods. The inset shows a higher magnification of the dashed rectangle, where the nanoribbon structure is clearly observed. The width of each individual nanoribbon is equal to four PCBM molecules. Scale bar 20 nm.

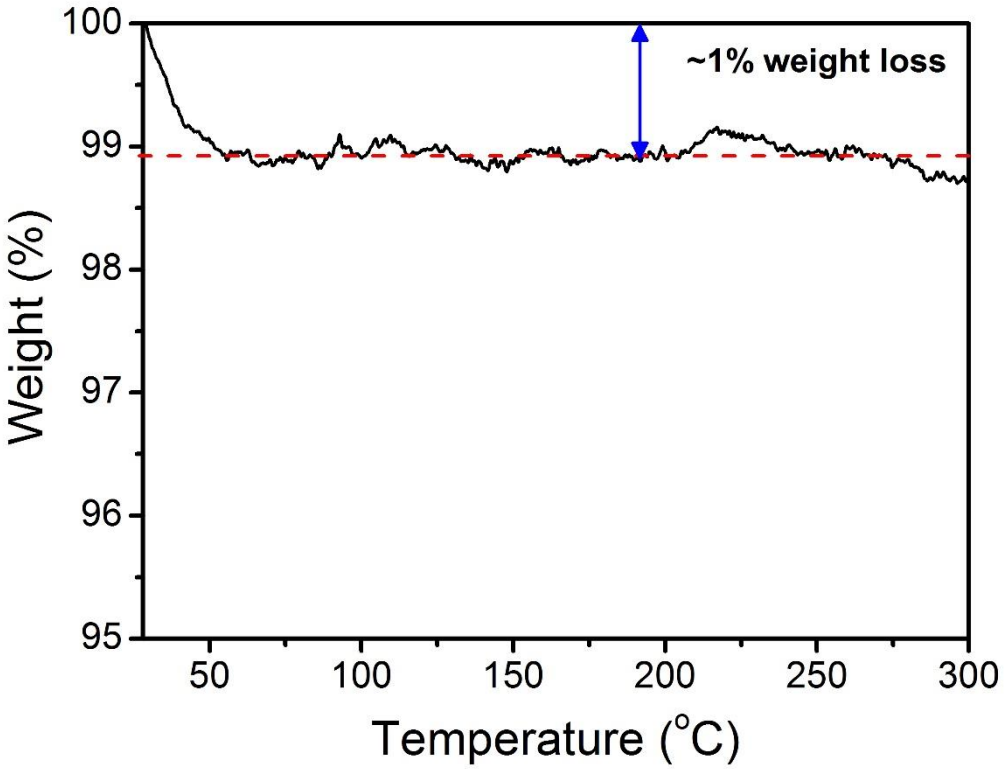

Figure S5. Thermogravimetric analysis of PCBM nanoribbons in nitrogen atmosphere, displaying a weight loss of about one percent up to 300 °C.

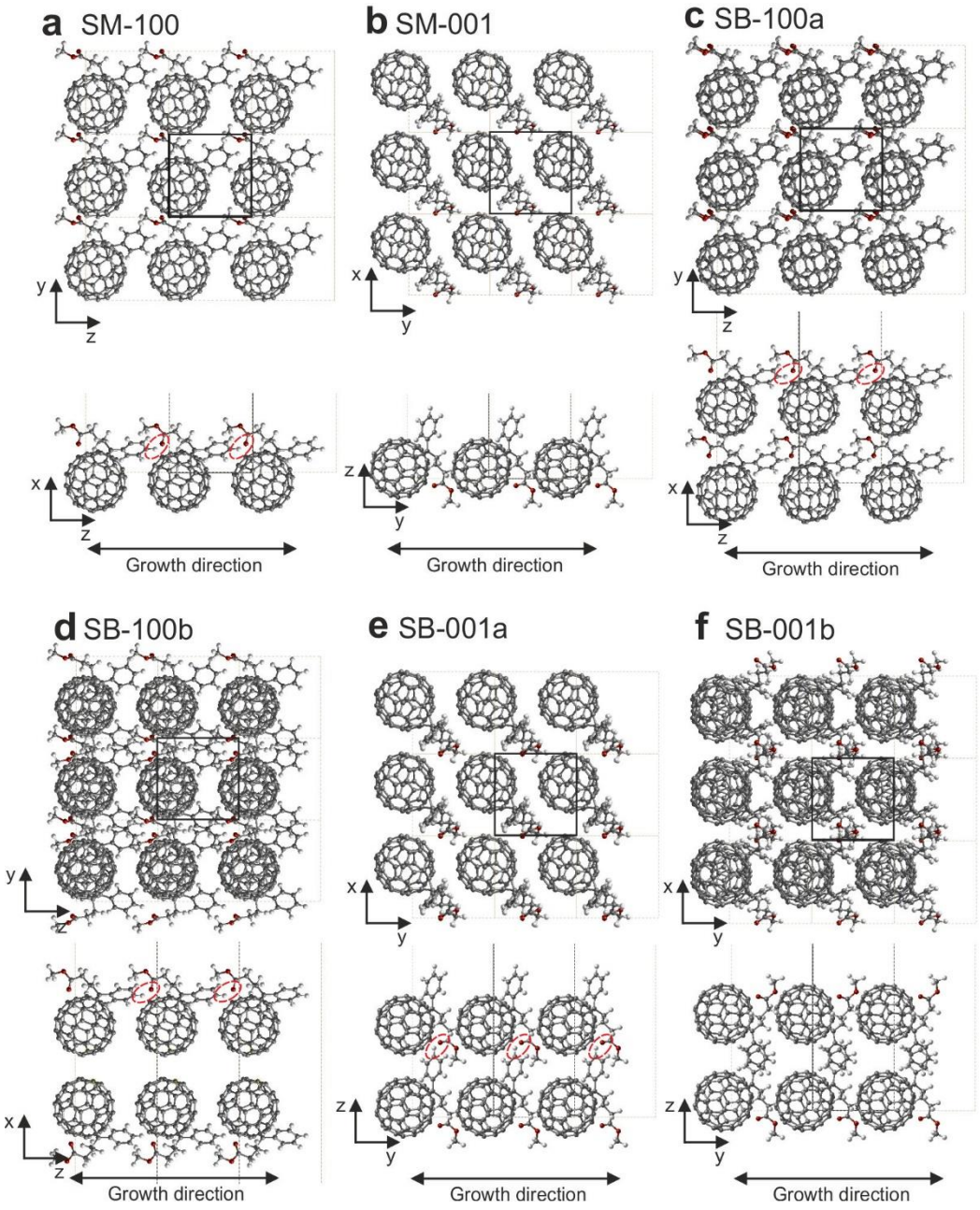

Figure S6. Top and side view of square PCBM monolayers and bilayers. **(a)** Square monolayer cut at the (100) crystal plane (labelled as SM-100). Note that in this case monolayers cut at (100) and (010) are equivalents. **(b)** Square monolayer cut at (001) crystal plane (labelled as SM-001), where the H-bond is not present resulting in a lower energetic stability. **(c)** Square bilayers cut along the (100) crystal plane with the side chains towards one direction. **(d)** Square bilayer where both tails points out of the structure. Note that a third configuration with both tails inside the bilayer is not easily obtained

due steric interactions between the functional groups. **(e-f)** Similar case for square bilayers cut at (001) plane.

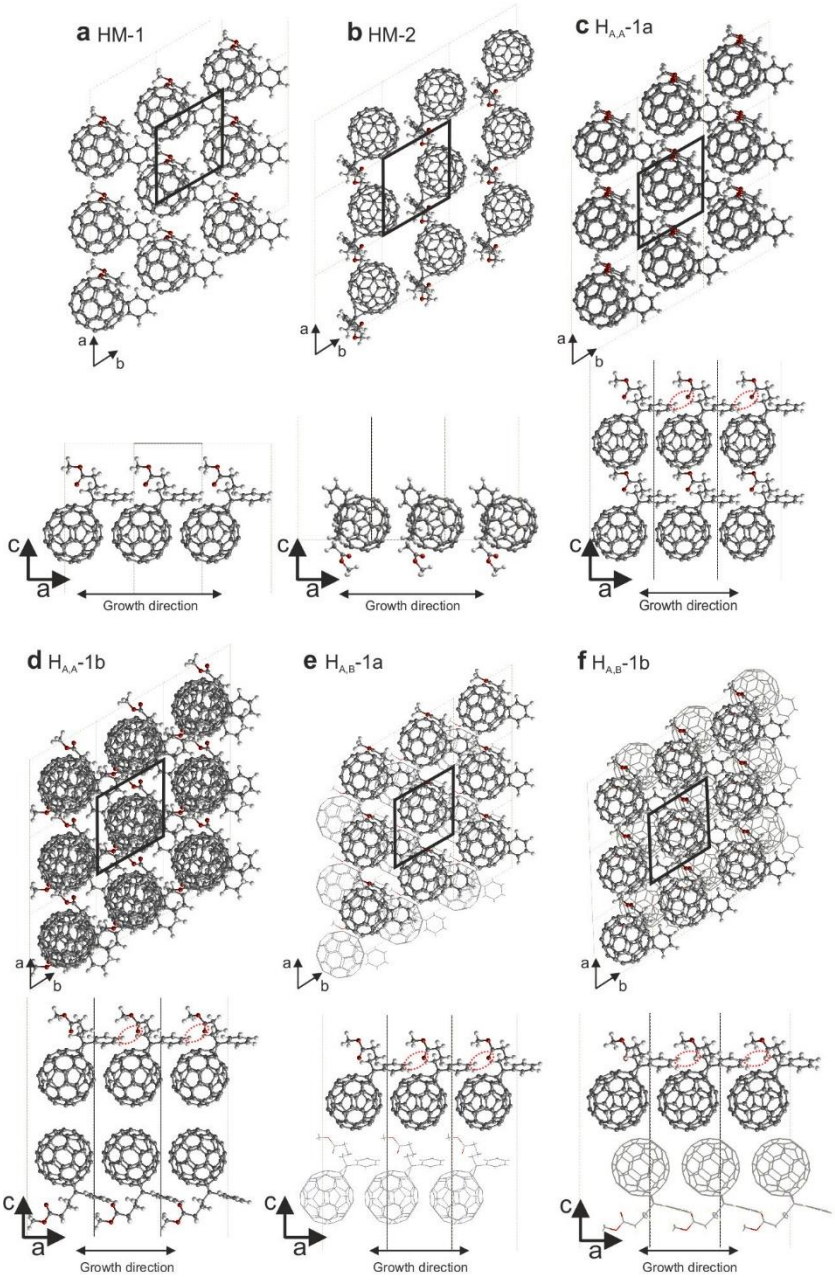

Figure S7. Top and side view of the hexagonal PCBM monolayers and bilayers. **(a)** A monolayer built with the side chains towards one side of the slab. **(b)** Monolayer with the side groups to the side of each PCBM, this configuration exhibit a larger lattice parameter, thus reducing the packing and interaction. **(c)** Hexagonal PCBM bilayer with "A-A" stacking with both side chains oriented towards

the same direction. **(d)** Hexagonal PCBM "A-A" bilayer with tails in different directions. **(e-f)** PCBM bilayer with an "A-B" stacking with the side chains towards the same **(e)** and contrary **(f)** directions.

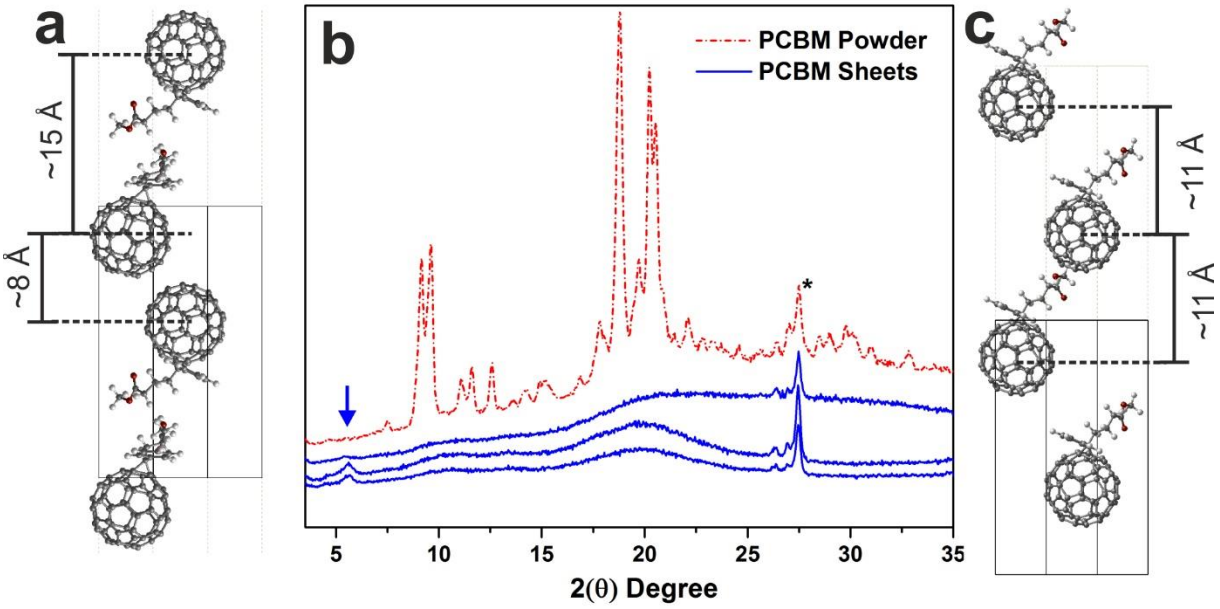

Figure S8. (a) Stacked configuration of PCBM bilayers as obtained from determined by dispersion-corrected DFT. (b) Experimental X-ray diffraction of bulk PCBM powder and 3 different batches of PCBM nanosheets. The diffractogram of the PCBM nanosheets exhibit similar peaks when compared to the bulk crystal, however a new feature is observed at ~5.6 degrees. This peak might be the results of a new inter-planar distance of 15 Å between stacked bilayers, as shown in (a). (c) Optimized bulk PCBM configuration with a hcp crystal structure. The star in (b) indicate the peak of the Si substrate.

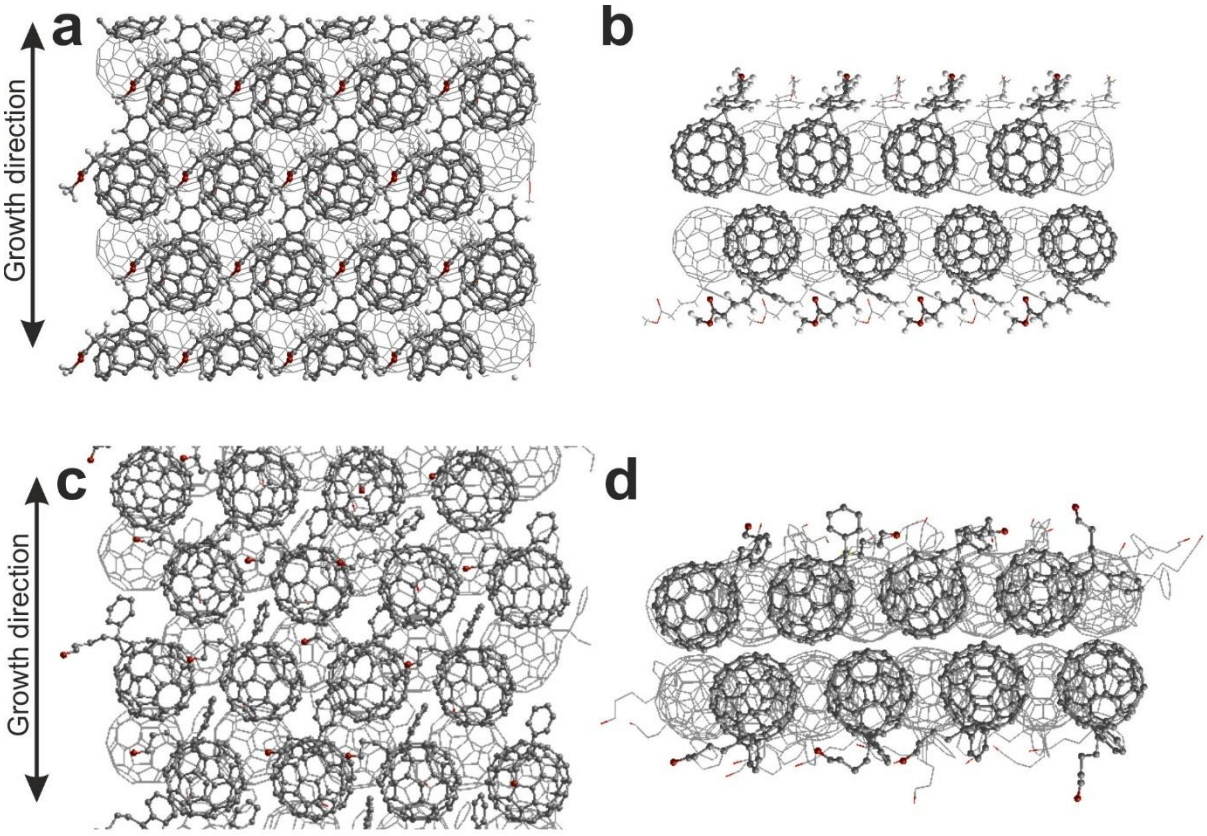

Figure S9. Top view and cross section of solvated PCBM nanoribbons. Initial **(a-b)** configuration obtained from DFT calculations, note the well-organized side chains. **(c-d)** Final snapshot of the molecular dynamics, now the side chains exhibit different orientations surrounding the PCBM nanoribbon and forming a micelle-like configuration. The solvent molecules and H atoms are omitted for clarity.