SUPPORTING INFORMATION

Transferring axial molecular chirality through a sequence of on-surface reactions

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Table of Contents

Experimental details: Sample preparation and STM imaging conditions.

- **Figure S1:** Chiral-dependent steric hindrance between enantiomeric radicals, illustrated with three-dimensional molecular models.
- Figure S2: Separation of enantioenriched monomers from racemic mixture via chiral HPLC.

Figure S3: Comparison of intermolecular distances (d_1 and d_2) in (*R*)- and (*S*)-polymers.

Figure S4: Comparison of chiral-dependent longitudinal end oblique orientation in (*R*)- and (*S*)- polymers.

Figure S5: (*R*)-polymer islands out of favored growth orientations.

- **Figure S6:** Constant-height maps with CO-functionalized tip of both (*pro-R*)- and (*pro-S*)-(3,1)cGNRs.
- **Figure S7:** Representative STM image and percentage of monomers chirality found in GNRs after polymerization of (*S*)-(-)-DBBA precursor.

Figure S8: Interspacing of (pro-*R*)- and (pro-S)-(3,1)-GNRs on Au(111) surface.

EXPERIMENTAL METHODS

Sample preparation. 2,2'-Dibromo-9,9'-bianthracene (DBBA) was synthesized following the procedure previously described.^[1] The enantiomers of DBBA were separated by HPLC (Agilent 1200) equipped with a chiral semipreparative column (Lux immobilized amylose-1; 4.6 x 250 mm, 5 μ m). The racemic mixture was separated using hexane:iPrOH (99:1) with a flow rate of 1.8 mL/min at 298 K (Fig S2). The optical rotations of each enantiomer were recorded on a JASCO P-2000 Polarimeter at 296 K using a sodium lamp (589 nm), obtaining a value of [α]_D = - 47.26 (c = 0.003, CH₂Cl₂) for the first HPLC peak and [α]_D = + 46.07 (c = 0.002, CH₂Cl₂) for the second HPLC peak. For the preparation of the different samples, the enantiomers of DBBA were independently evaporated at 435 K from a home-made Knudsen cell oriented towards the monocrystalline Au(111) surface substrate for deposition. Atomically cleaned Au(111) surface were obtained by standard sputtering (0.8 kV, Ar⁺) and annealing cycles (705K). Thermally-induced on-surface reactions were performed by radiative heating, at 415K (525K) for Ullmann coupling (cyclodehydrogenation).

STM imaging and analysis. Sample analysis was performed in a commercial Scienta-Omicron low-temperature STM under ultrahigh vacuum (UHV) conditions with pressure values below the 10⁻¹⁰ mbar range and a base temperature of 4.3 K. All STM images were processed with the WSxM software.^[2]The chirality determination from the STM images was performed as described in the text, and the provided statistics are the result of counting the number of monomer units (each accounting for one unit cell in polymers and GNRs) observed in polymers or GNRs of each handedness. For larger scale images, once the chirality of a polymer or GNR is determined, the number of monomers is estimated from the polymer/GNR length divided by the respective unit cell size. The reported errors stem from the square root of the total monomer counts for each species and chirality. The total number of monomers considered in the statistics amount to 7200, 2077 and 2150 in the samples corresponding to the enantioenriched S-reactants in the polymer phase, enantioenriched S-reactants in GNR phase, and the control experiment with enantioenriched R-reactants in GNR phase, respectively.



Fig. S1. 3D models illustrating the steric hindrance exerted between dehalogenated monomers of (a) the same and (b) different chirality. The latter displays a strong steric hindrance that hinders polymerization of monomers with opposite chirality.



Fig. S2. Chiral HPLC profiles for (top) DBBA racemate, and enantiomerically enriched (middle) (S)-(+)- and (bottom) (R)-(-)-DBBA precursors.



Fig. S3. Identification of the polymer's chirality from their non-equivalent intramolecular distances between the uppointing ends of the tilted anthracene moieties. Examples (a) (S)-polymer and (b) (R)-polymer (Vs = 0.5 V, It = 10-50 pA).



Fig. S4. Identification of the polymer's chirality from their longitudinal end oblique orientation. Examples ($V_s = 0.5 \text{ V}$, $I_t = 50 \text{ pA}$) of (a) (*S*)-polymer and (b) (*R*)-polymer with superimposed models where, for an easier visualization, just terminal hydrogen atoms (in white) are represented.



Fig. S5. STM images ($V_s = 1.0 \text{ V}$, $I_t = 32 \text{ pA}$) showing examples of (*S*)-polymers islands out of main growth orientations (circled in white dashed lines).



Fig. S6. Constant-height current maps ($U_s = 2 \text{ mV}$, color scale on the right) with a CO-terminated tip showing (a-c) (*pro-S*)-GNRs and (d-f) (*pro-R*)-GNRs in their three growth orientations on Au(11), as indicated in the central inset.



Fig. S7. a) Representative STM overview image ($V_s = 0.1$ V, $I_t = 50$ pA) of the sample after depositing enantioenriched (*R*)-(-)-DBBA precursor and inducing its polymerization and cyclodehydrogenation. White dashed lines represent the boundaries of the herringbone reconstruction domains that determine the preferred orientations of GNRs. Inset indicates the preferred adsoption orientations of prochiral GNRs with respect to Au(111) . b) Enantiomeric distribution of the monomers forming the GNRs after polymerization and cyclodehydrogenation of enantioenriched (*R*)-(-)-DBBA precursors.



Fig. S8. STM images ($V_s = 1.0V$, $I_t = 200pA$; $V_s = 0.5V$, $I_t = 150pA$) showing the well-defined preferred interspacing observed for both (a) (*pro-S*)-GNRs and (b) (*pro-R*)-GNRs. Green lines correspond to the height profiles at the bottom of each image. Dashed black lines indicate the height profile directions.

References

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