

Electronic Supplementary Information (ESI)

Interaction-site model prediction of molecular self-organization on $p2$ -substrate symmetry

C. Rohr,^{*a} M. Balbás Gamba,^b K. Gruber,^a C. Höhl,^a M. Malerek,^c L. Scherer,^c
E. C. Constable,^c T. Franosch,^{b,d} B.A. Hermann^{*a}

^a Center for Nano Science (CeNS) and Walther-Meissner-Institute of Low Temperature Research of the Bavarian Academy of Sciences, Walther-Meissner-Str. 8, 85748 Garching, Germany

^b Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nano Science (CeNS), Department of Physics, LMU München, Theresienstraße 37, 80333 München, Germany

^c Department of Chemistry, University of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

^d Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

E-Mail: b.hermann@cens.de

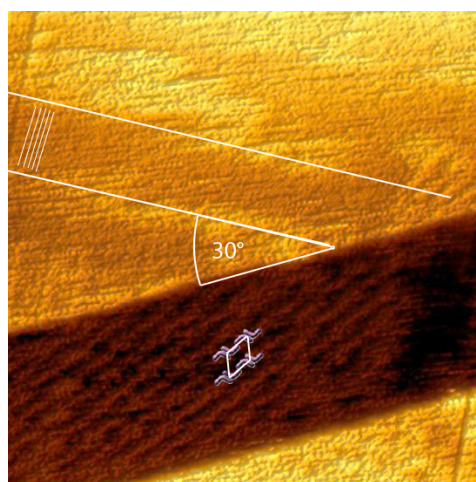


Fig.S1: “Wave” ordering of Fréchet-dendrons on pentacontane imaged by STM. Rarely observed “wave” domain is visible in the dark brown graphite depression. The schematic ordering is indicated with the unit cell and schematic molecular backbones. Slightly visible are adjacent pentacontane rows on the higher graphite terraces (yellow area) indicated by the white lines. The pentacontane rows have the characteristic 30° angle with respect to the graphite substrate. Parameters: a) $U_{\text{Bias}} = -800$ mV, $|I_T| = 0.3$ pA, 40 nm x 40 nm.

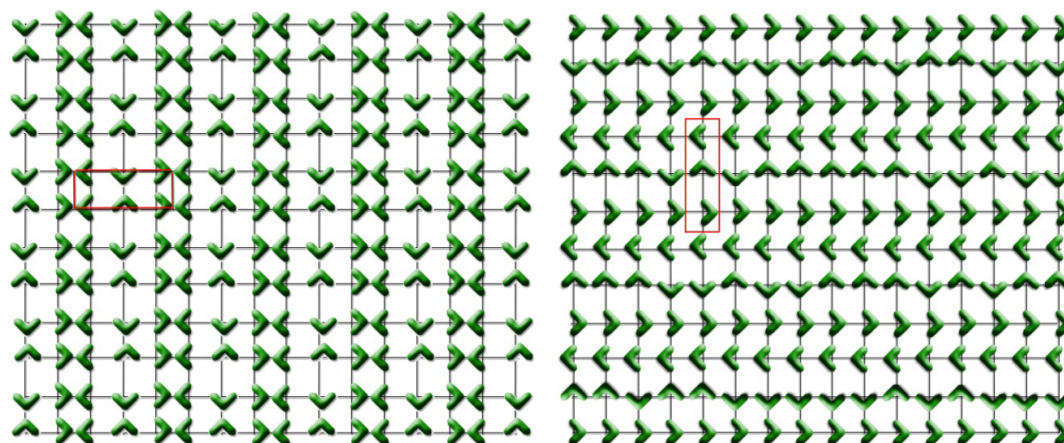


Fig.S2: Monte-Carlo simulated interlaced ordering motifs. (a) Second interlaced “jigsaw” structure found for conformer ζ . The interlacing molecules have a fixed orientation (b) Interlaced “tiretrack” structure found for conformer ϵ with interlacing rows of non-fixed orientation.