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Article

Fingerprints of sp^1 Hybridized C in the Near-Edge X-Ray Absorption Spectra of Surface-Grown Materials
Supplementary Materials

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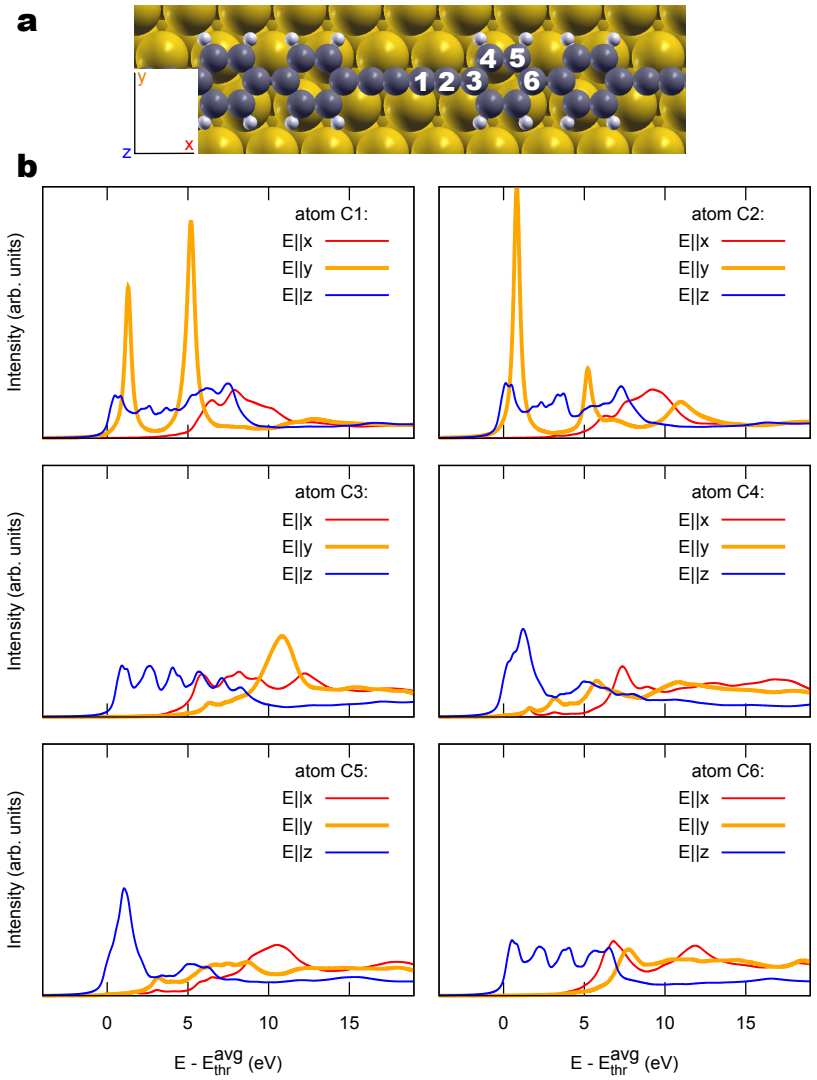

Figure S1. (a) Structural model and inequivalent carbon atoms in bBEBP/Au(111). (b) Decomposition of the NEXAFS spectrum of bBEBP/Au(111) into the individual initial-state contributions, as numbered in panel (a).

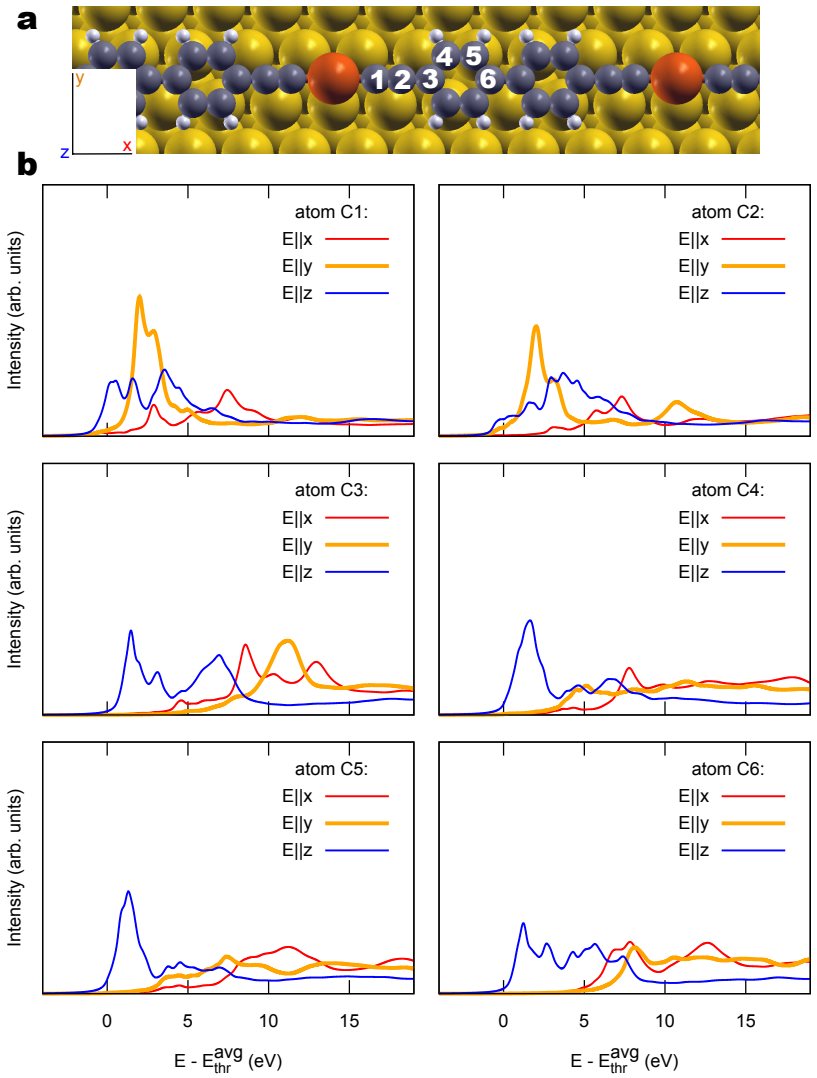

Figure S2. (a) Structural model and inequivalent carbon atoms in bBEBP/Au(111) embedding a Au adatom (red) in between two organic units. (b) Decomposition of the corresponding NEXAFS spectrum into the individual initial-state contributions, as numbered in panel (a).

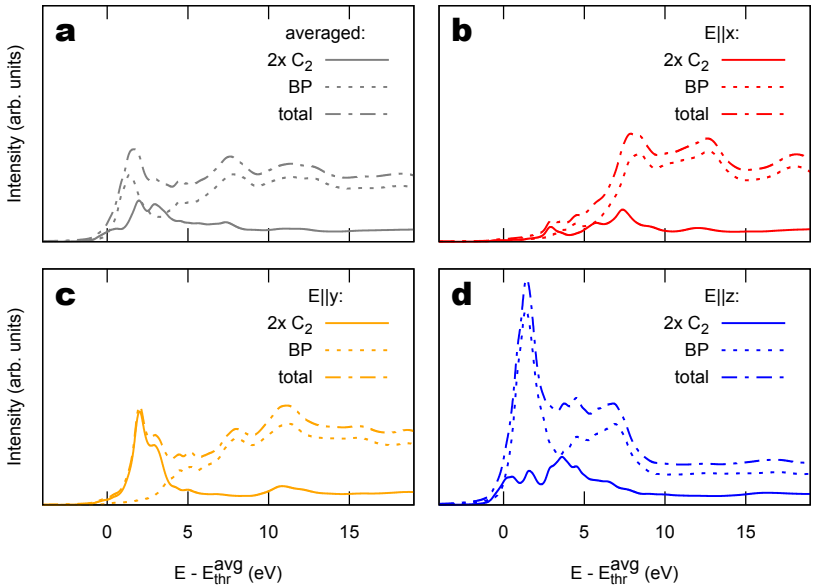

Figure S3. Decomposition of the NEXAFS spectrum of bBEBP/Au(111) embedding a Au adatom on contributions by the sp^2 biphenyl part (BP) and the sp^1 chains (C_2). (**a**) Spectrum averaged over the polarizations. (**b**) In-plane electric field along the polymer axis x and (**c**) orthogonal to it, y; (**d**) out-of-plane electric field, z. See Figure S2a for the definition of x, y, z axes.

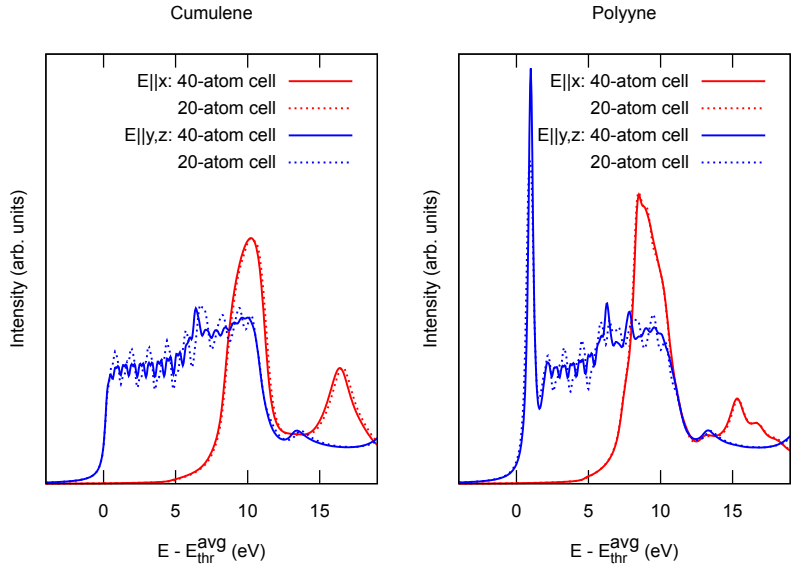

Figure S4. NEXAFS spectrum of cumulenes (left) and polyynes (right) computed with a 20-atom and 40-atom simulation supercell. One atom per cell is excited. Polarization directions are taken with x along the chain axis and y, z orthogonal to it.