

Electronic supplementary information (ESI) for Nanoscale

Preservation of the donor-acceptor character of a carbazol-phenalenone dyad upon adsorption on Pt(111)

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S1: STM overview of a prototypical Pt(111) surface after CBHP evaporation

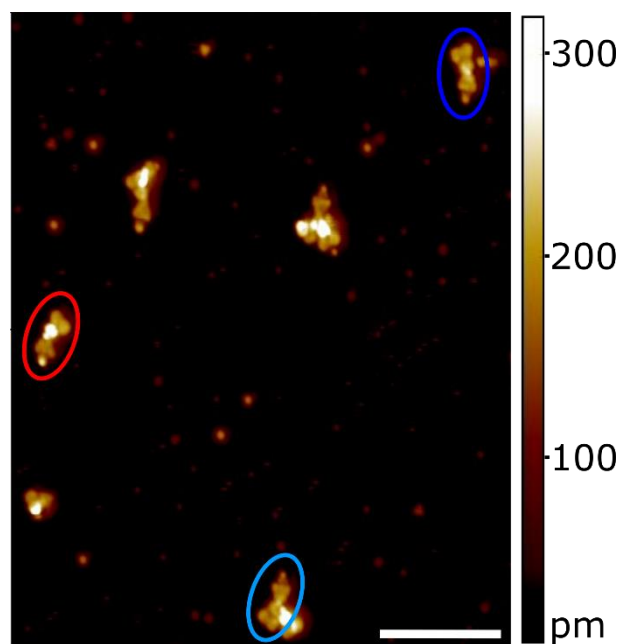


Fig. S1 STM image ($U_{\text{BIAS}} = 50$ mV, $I_{\text{SET}} = 200$ pA, scale bar = 5nm) showing a typical sample of CBHP adsorbed on Pt(111). Two different adsorption configurations, ConA marked by a blue and ConB by a red ellipse, can be assigned to single molecules. One of the mirror configurations of CBHP, ConA', is exemplarily marked by a light blue ellipse. A recurring type of fragment, consisting of three spots, one bright and two shallow, is observed below CBHP in configuration ConB. These fragments often show up close to our target molecules (see center of Fig. S1).

S2 and S3: Detailed measurements of CBHP dimensions in ConA and ConB

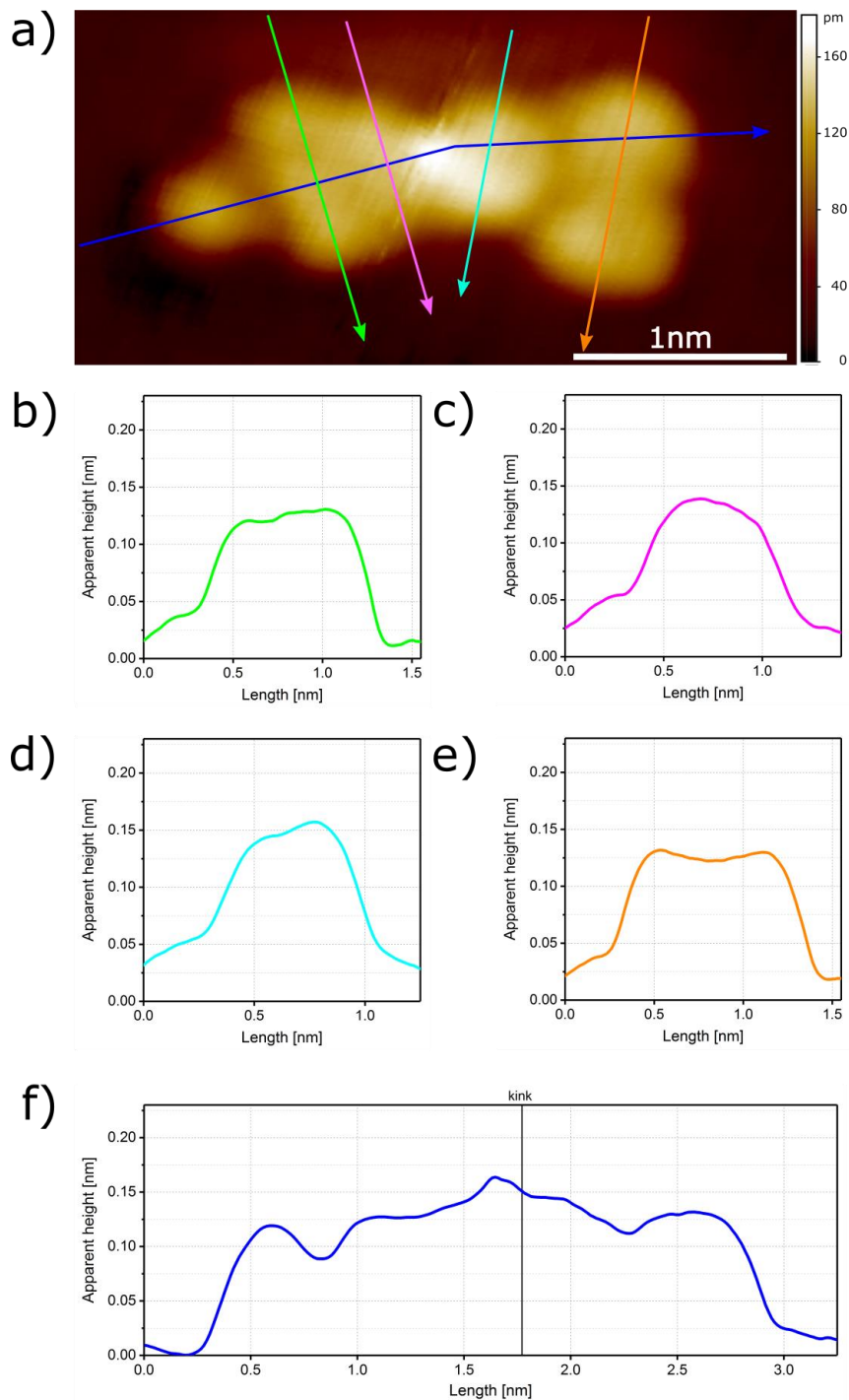


Fig. S2 (a) Unfiltered high resolution STM measurement ($U_{\text{BIAS}} = 50$ mV, $I_{\text{SET}} = 200$ pA) of Fig. 1a. An identical color scale is used in Fig. S3a. (b–f) Averaged apparent height profiles along different directions of configuration ConA of CBHP. Direction and position of the corresponding height profiles are given in a) in the same color scheme. (f) This profile follows a kink along the molecular axis.

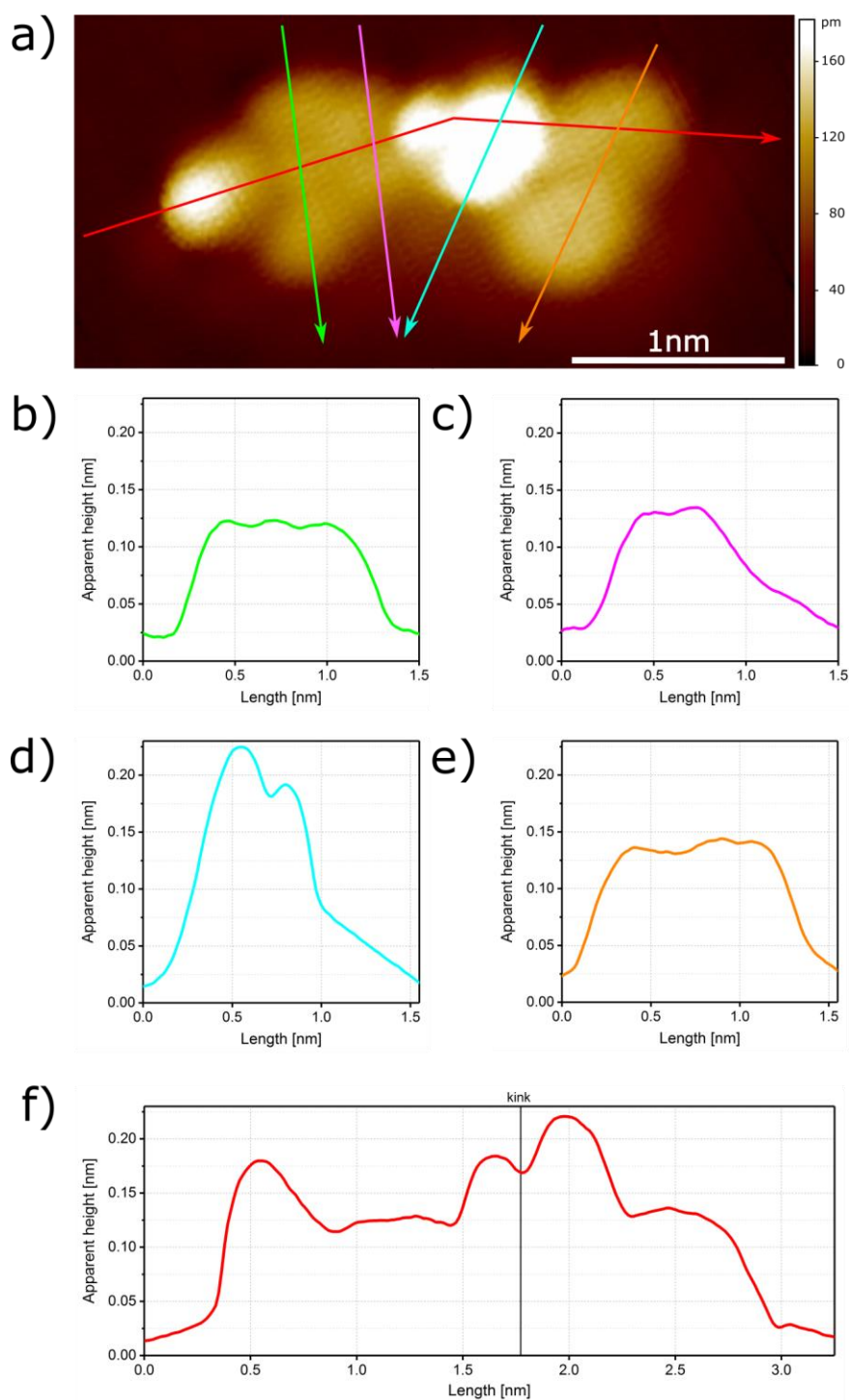


Fig. S3 (a) Unfiltered high resolution STM measurement ($U_{\text{BIAS}} = 50$ mV, $I_{\text{SET}} = 200$ pA) of Fig. 1b. An identical color scale is used in Fig. S2a. (b–f) show averaged apparent height profiles along different directions of configuration ConB of CBHP. Direction and position of the corresponding height profiles are given in a) in the same color scheme. (f) This profile follows a kink along the molecular axis.

S4: Calculated geometries and STM images of CBHP on Pt(111)

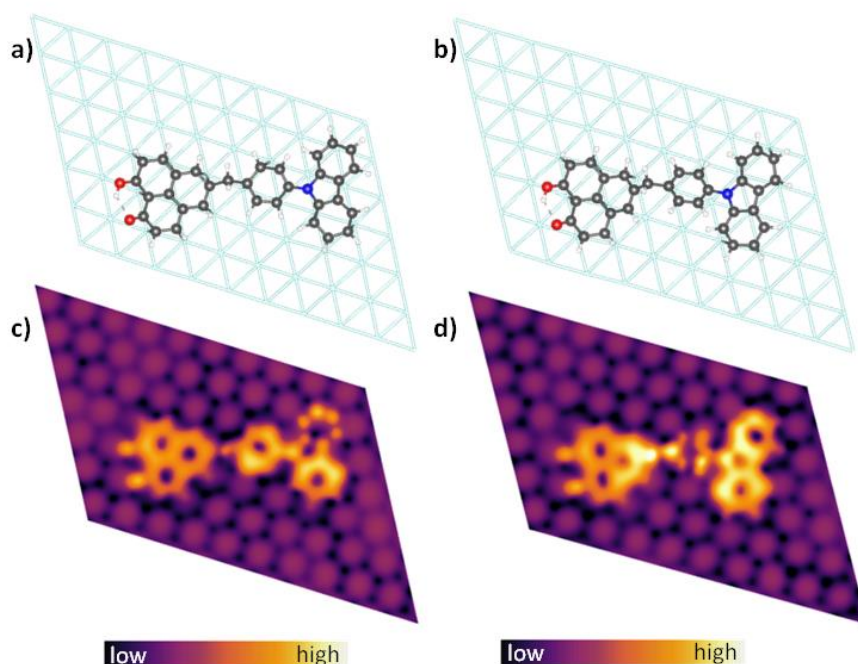


Fig. S4 (a, b) Geometries of the CBHP molecule, where no Pt adatom is present, on the Pt(111) surface corresponding to local minima from DFT calculations (c, d) Simulated constant-current STM images around the Fermi energy.

S5: Progress of a raw to a filtered STM image

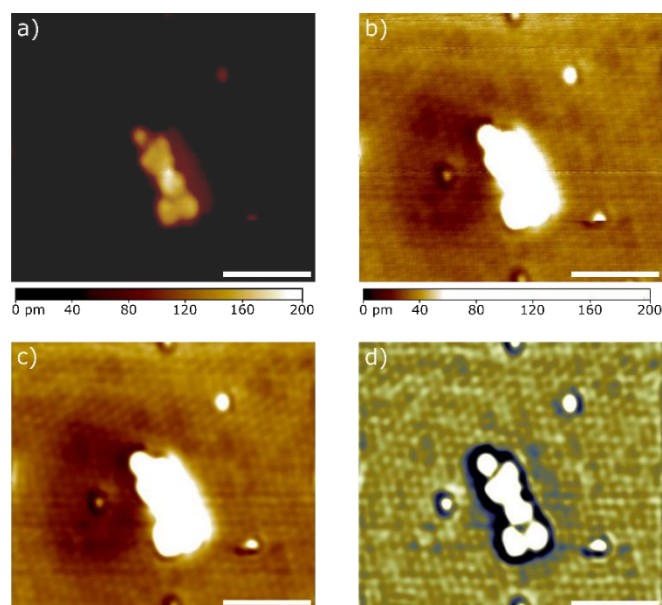


Fig. S5 Steps of image processing for Fig. 2a to present the atomic structure of the Pt(111) substrate combined with orbital molecular features of CBHP in the same STM image. (a, b) Raw STM measurements of a single molecule in ConA in different apparent height scales. The scale in a) puts the focus on the molecular structure while the scale chosen in b) emphasizes the atomic lattice of Pt(111). (c) Slight Fourier filtering of b) reduces the noise. (d) In a last step an ISO 11562 Gaussian Profile Filter is applied to c).

S6: Voltage dependent STM images of CBHP in ConA

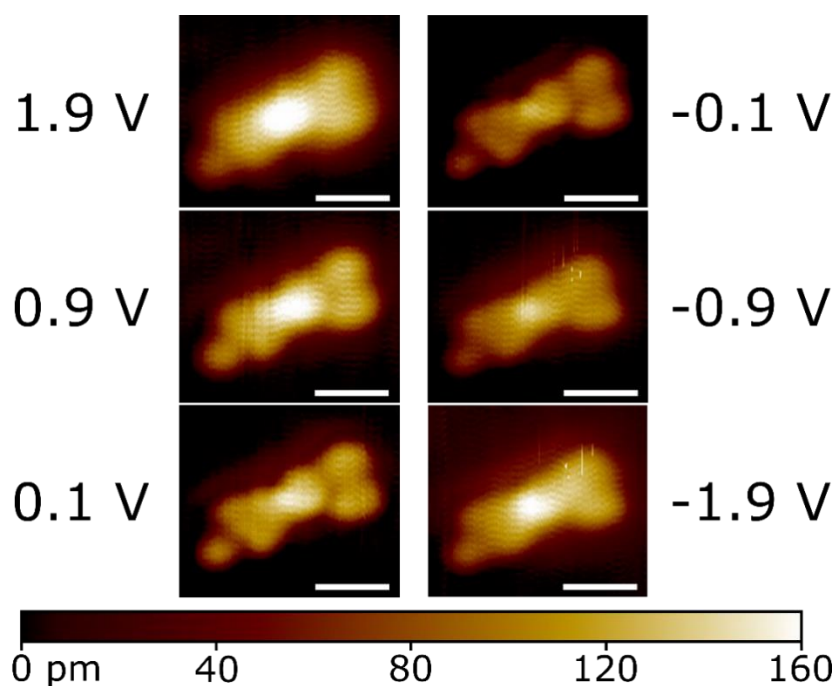


Fig. S6 Voltage dependent STM measurement ($I_{\text{SET}} = 200$ pA) of ConA. An identical color scale is used for all unfiltered Images. The scale bar is 1 nm.

S7: PDOS of ConA together with LDOS at selected energies

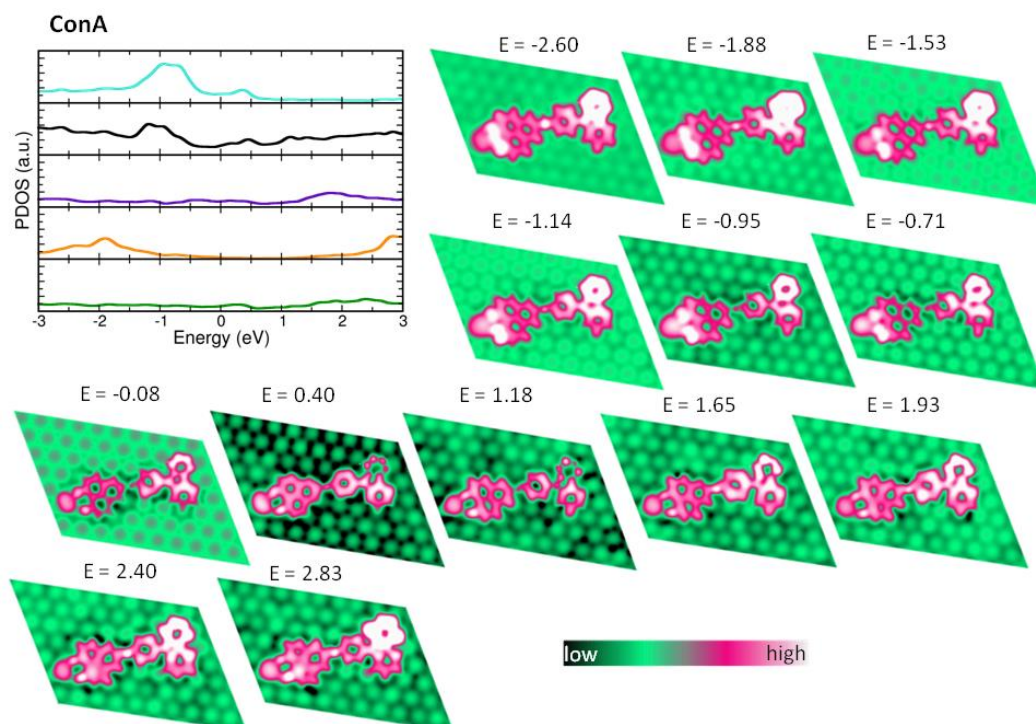


Fig. S7 Calculated PDOS of the CBHP-Pt donor-acceptor dyad adsorbed in ConA and LDOS at selected energies (in eV). Color code like indicated in Fig. 3 and 4: HP acceptor (black), central part (purple), two spots over the donor CB (green and orange), Pt adatom (turquoise).

S8: Kohn-Sham frontier molecular orbitals (FMOs) for CBHP in acetonitril

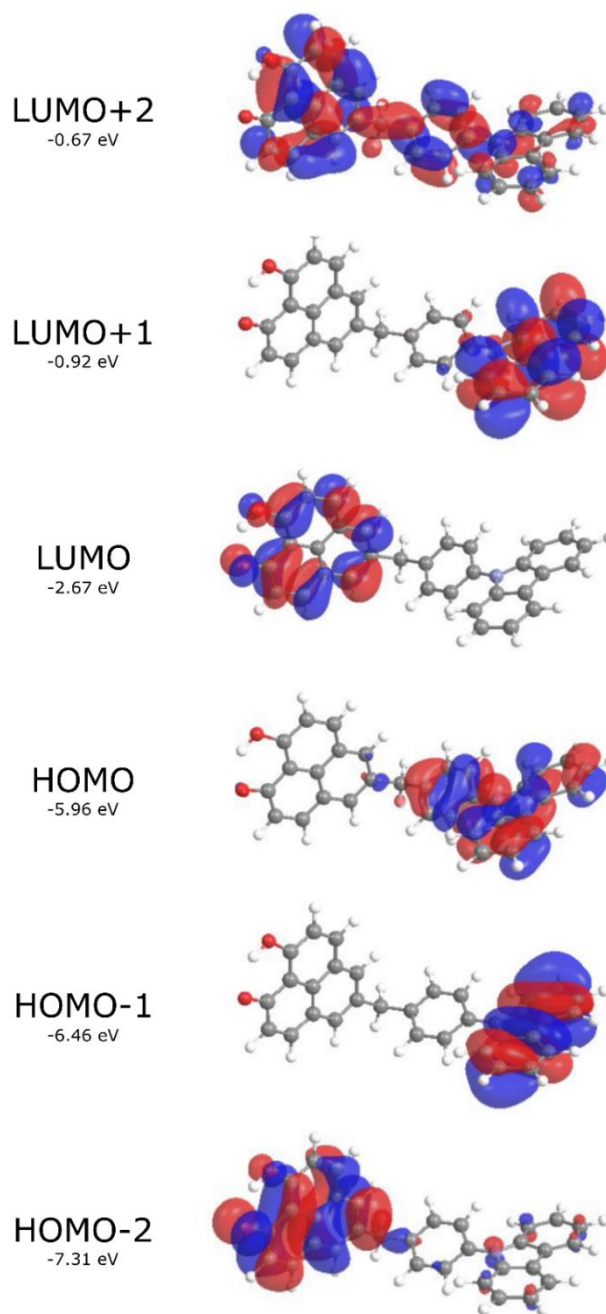


Fig. S8: Chosen Kohn-Sham Frontier Molecular Orbital (FMOs) for CBHP. A polarizable continuum model was used for its calculation (*Gaussian 09 PBEh1PBE/6-311+G***) with acetonitrile as solvent.

S9 and S10: Frontier molecular orbitals of CBHP and CBHP-Pt in ConA and ConB

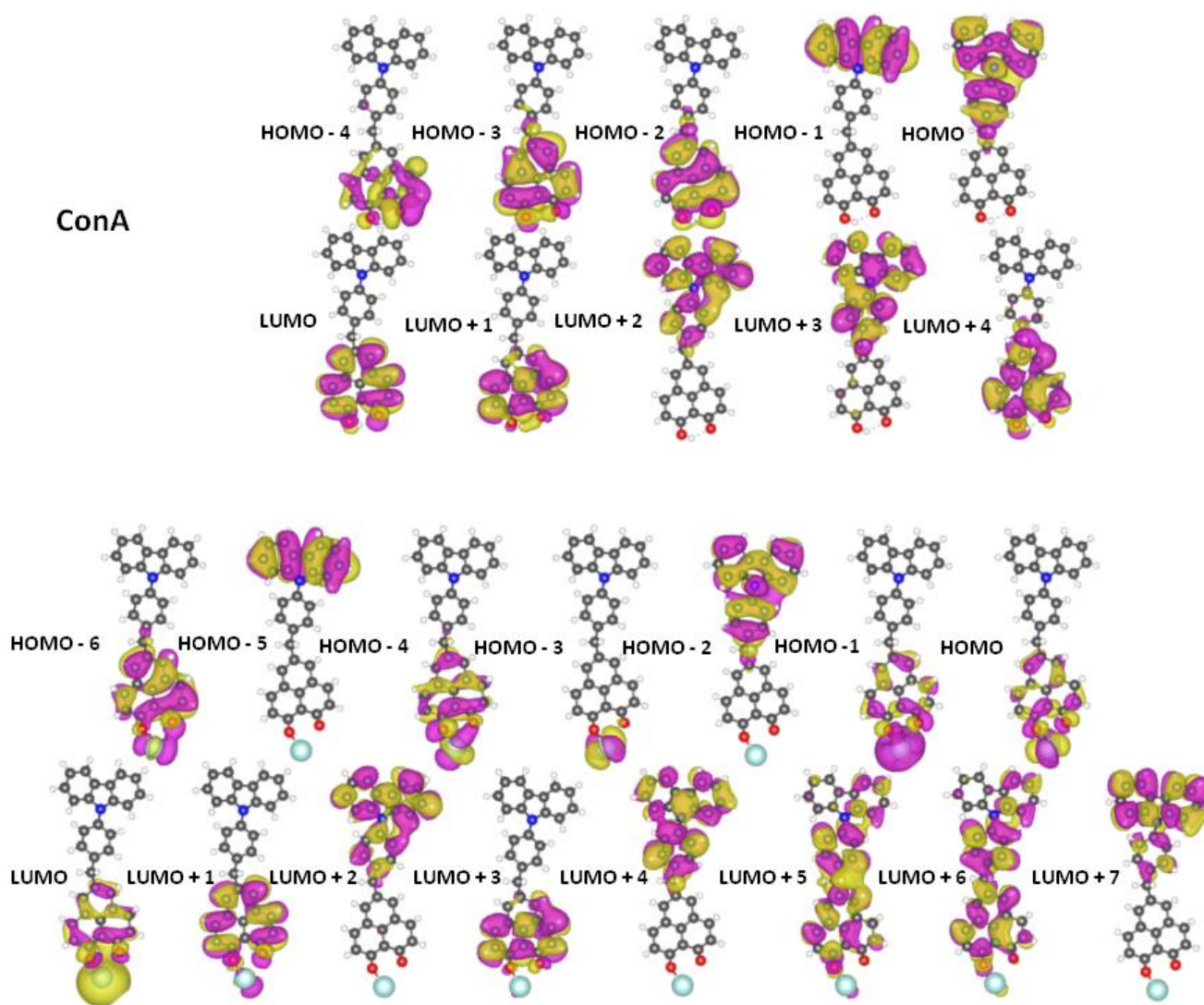


Fig. S9 Occupied and unoccupied frontier molecular orbitals of the isolated CBHP molecule (top) and of the CBHP-Pt complex (bottom) in ConA.

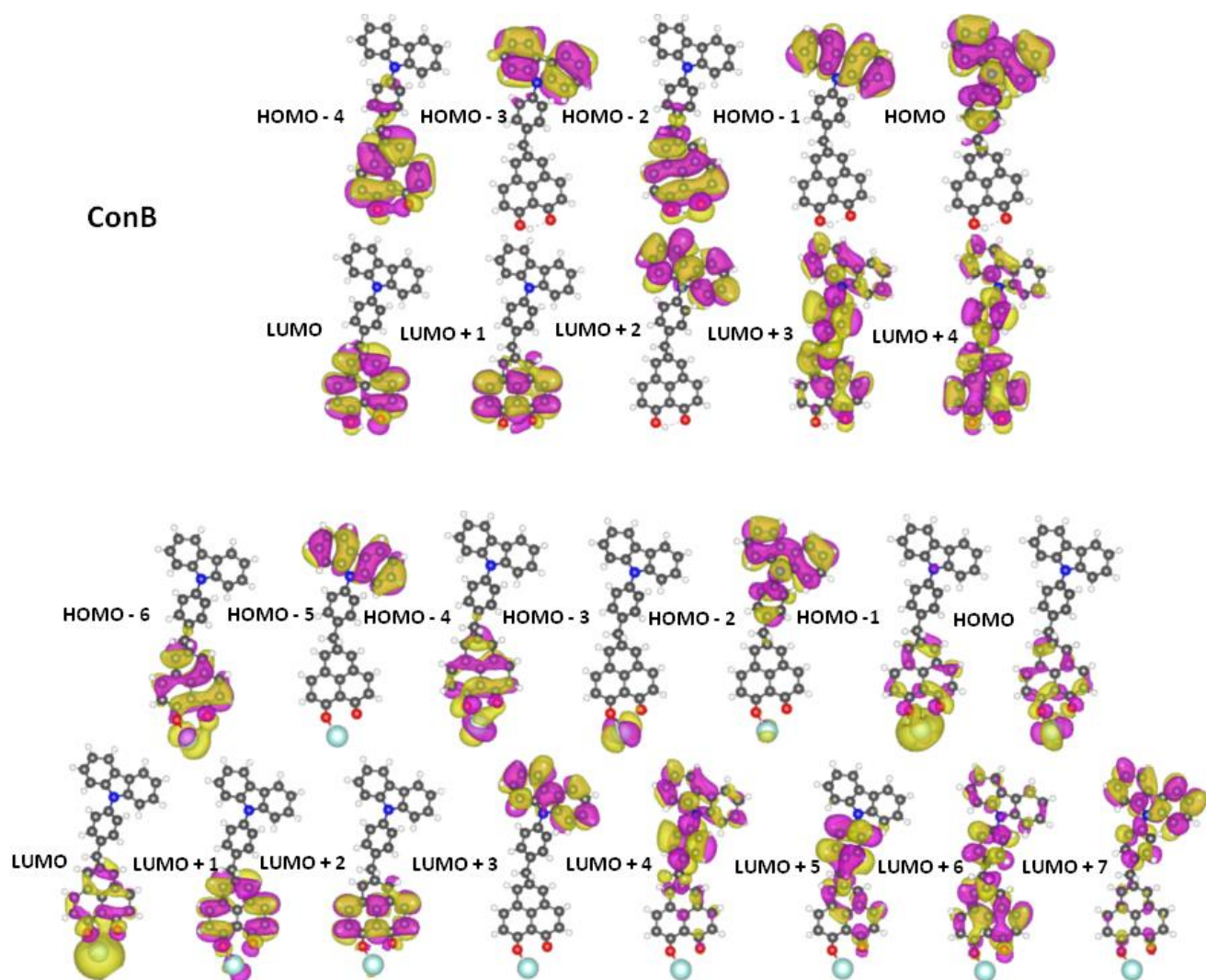


Fig. S10 Occupied and unoccupied frontier molecular orbitals of the isolated CBHP molecule (top) and of the CBHP-Pt complex (bottom) in ConB.

S11: PDOS of ConB together with LDOS at selected energies

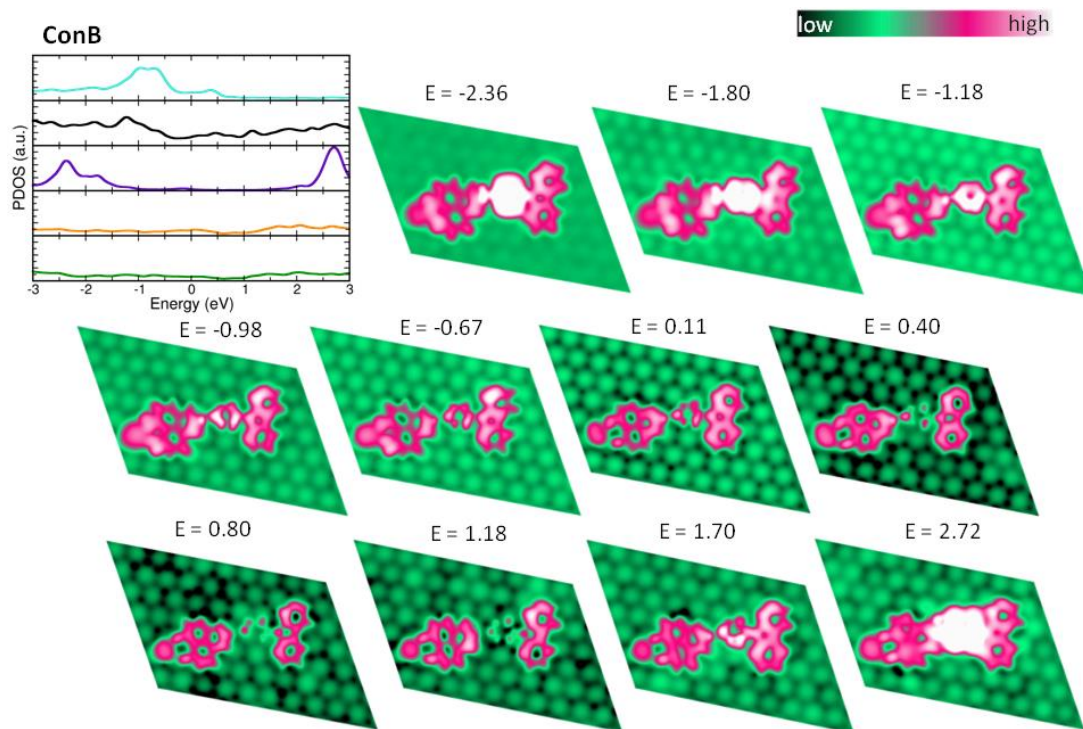


Fig. S11 Calculated PDOS of the CBHP-Pt donor-acceptor dyad adsorbed in ConB and LDOS at selected energies (in eV). Color code like indicated in Fig. 3 and 4: HP acceptor (black), central part (purple), two spots over the donor CB (green and orange), Pt adatom (turquoise).

S12: TGA and DTA of CBHP

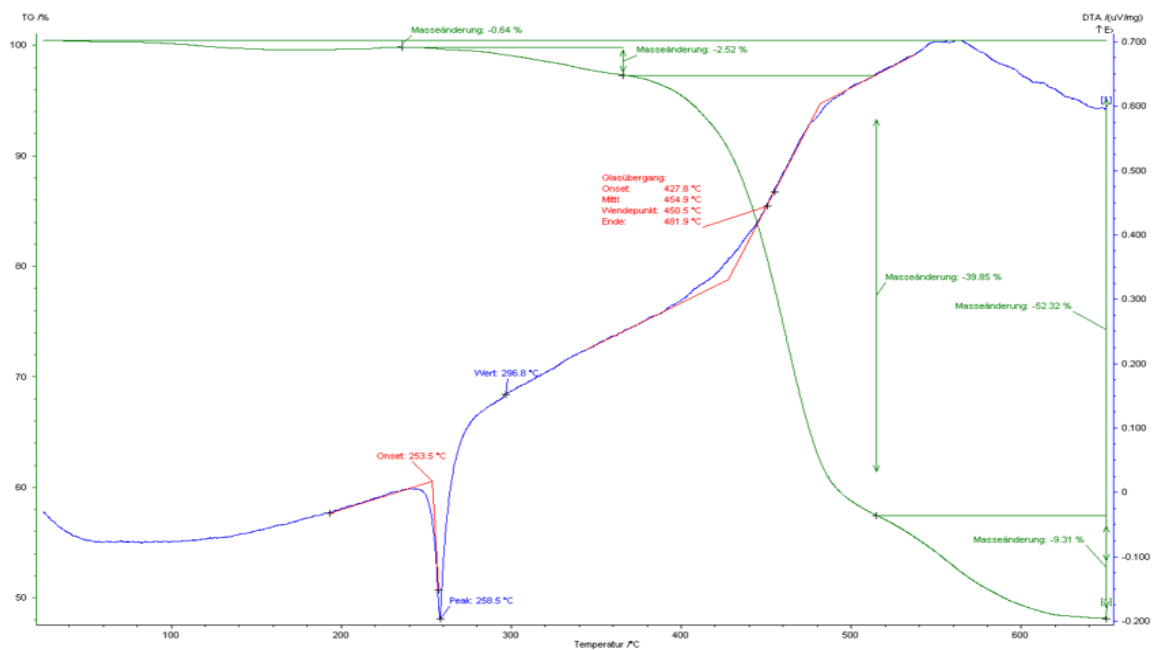


Fig. S12: Thermogravimetric (TGA) and differential thermal analysis (DTA) of CBHP measured using simultaneous thermal analyzer NETZSCH STA 449C.