Supporting Information for: Quantitative Electronic Structure Determination of N-Heterotriangulene Derivatives Adsorbed on Au(111)

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1 Two-photon photoemission data of *N*-HTA-550 adsorbed on Au(111)

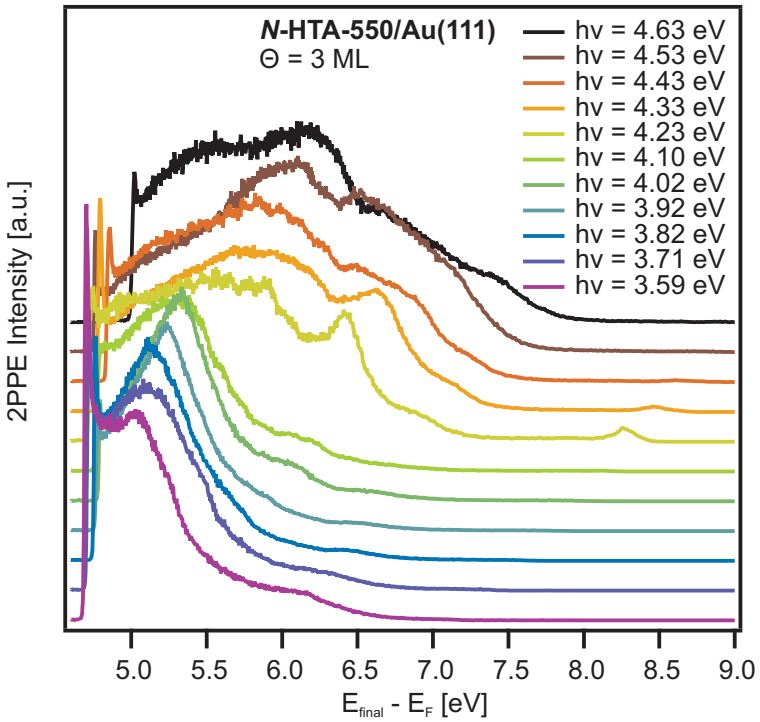

Figure S1: Photon energy dependent 2PPE spectra of 3 ML *N*-HTA-550 adsorbed on Au(111). The energy axis reveals the final state (E_{Final}) of photoemitted electrons with respect to the Fermi energy E_F ($E_{Final} - E_F = E_{kin} + \Phi$); thus, the low-energy cutoff corresponds to the work function (Φ) of the adsorbate/substrate system.

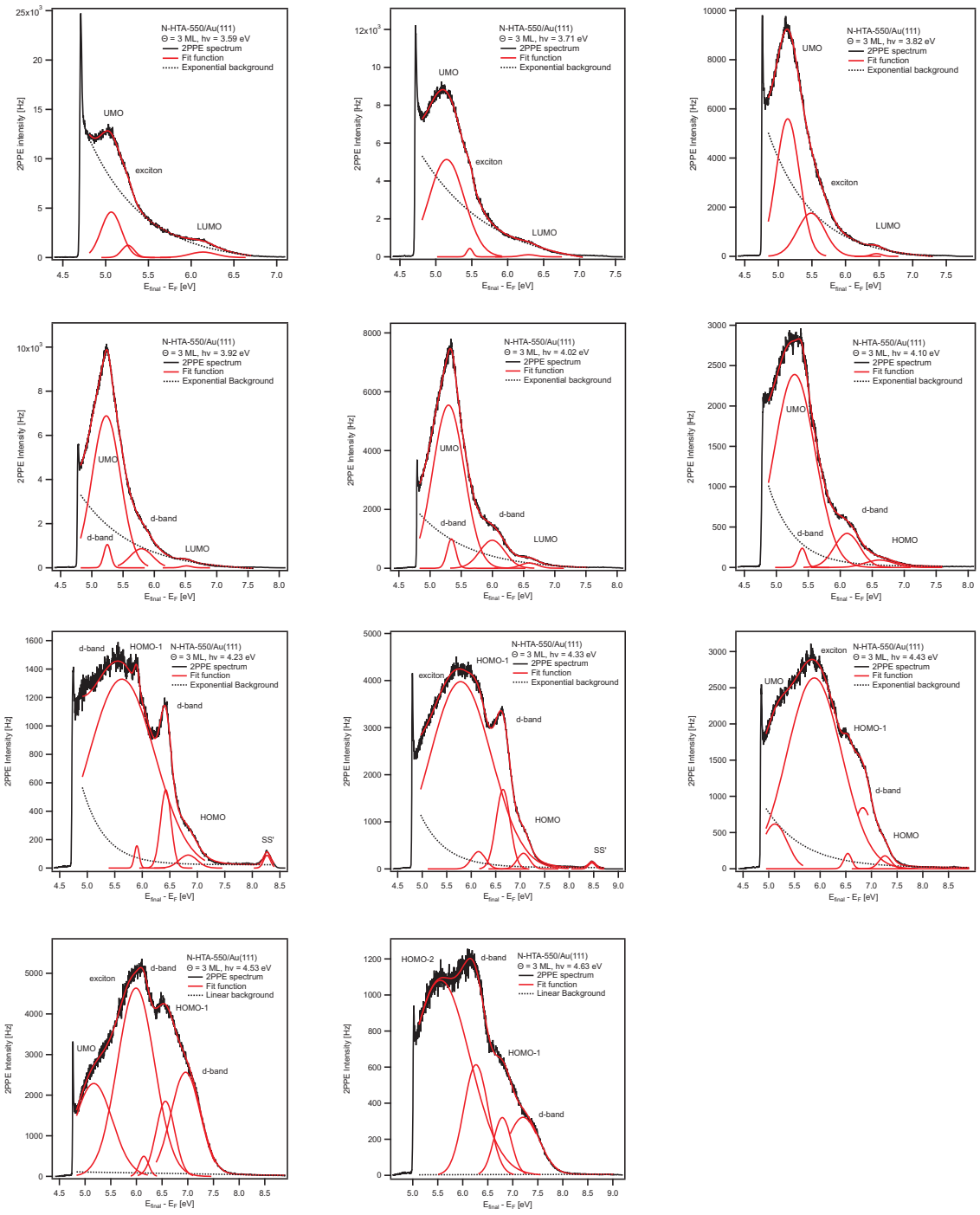

Figure S2: Photon energy dependent 2PPE spectra of 3 ML *N*-HTA-550 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves).

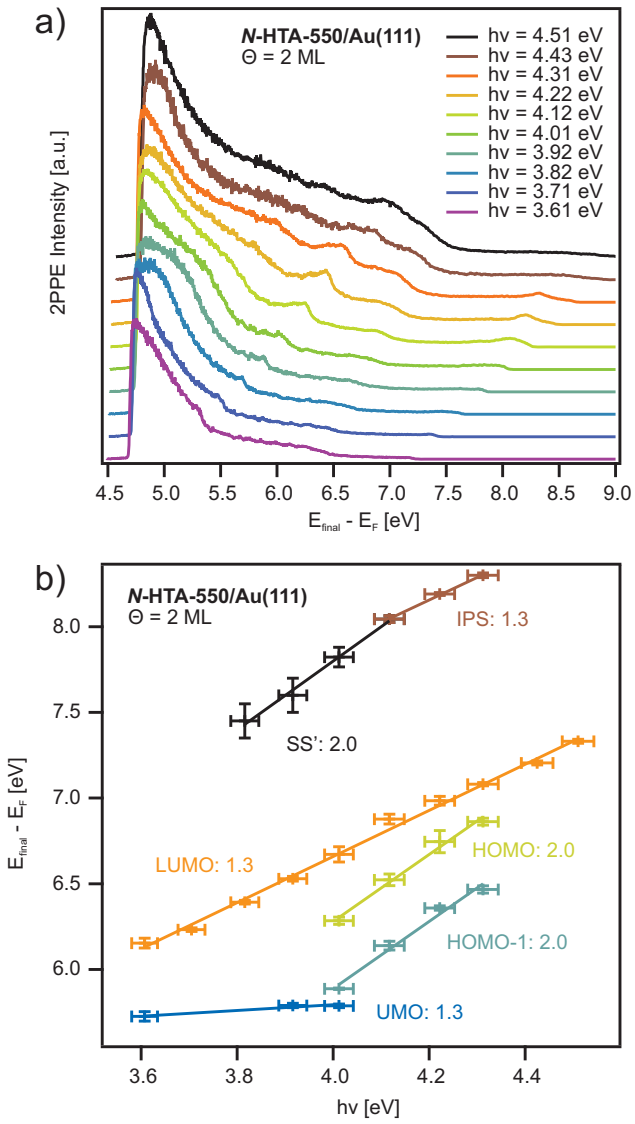

Figure S3: a) Photon energy dependent 2PPE spectra of 2 ML *N*-HTA-550 adsorbed on Au(111). b) Photon-energy-dependent peak position extracted to assign peaks observed in the 2PPE spectrum to occupied, unoccupied intermediate or final electronic states. A slope of 1 suggests that a peak originates from an unoccupied intermediate state, a slope of zero from an unoccupied final state (located above the vacuum level), while a slope of 2 is related to peaks originating from occupied states. The slopes from the fits are given next to the respective data (UMO: unoccupied molecular orbital; IPS: image potential state; SS: surface state).

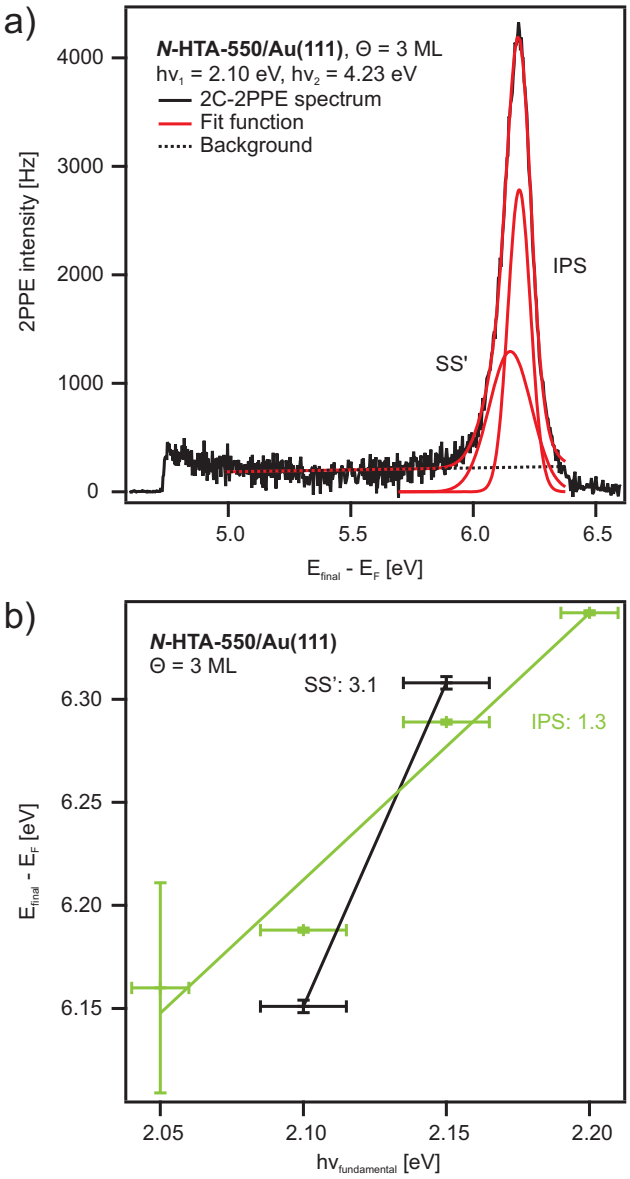

Figure S4: a) Two-color 2PPE spectrum of 3 ML *N*-HTA-550 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves; IPS: image potential state; SS: surface state). b) Photon-energy-dependent peak position extracted to assign peaks observed in the 2PPE spectrum to occupied and unoccupied intermediate electronic states. The slopes from the fits are given next to the respective data.

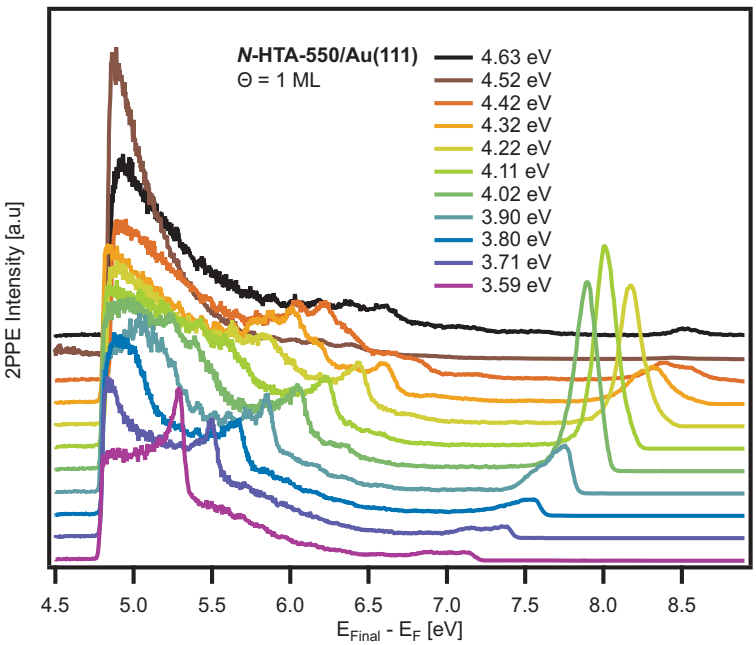

Figure S5: Photon energy dependent 2PPE spectra of 1 ML *N*-HTA-550 adsorbed on Au(111). The energy axis reveals the final state (E_{Final}) of photoemitted electrons with respect to the Fermi energy E_F ($E_{Final} - E_F = E_{kin} + \Phi$); thus, the low-energy cutoff corresponds to the work function (Φ) of the adsorbate/substrate system.

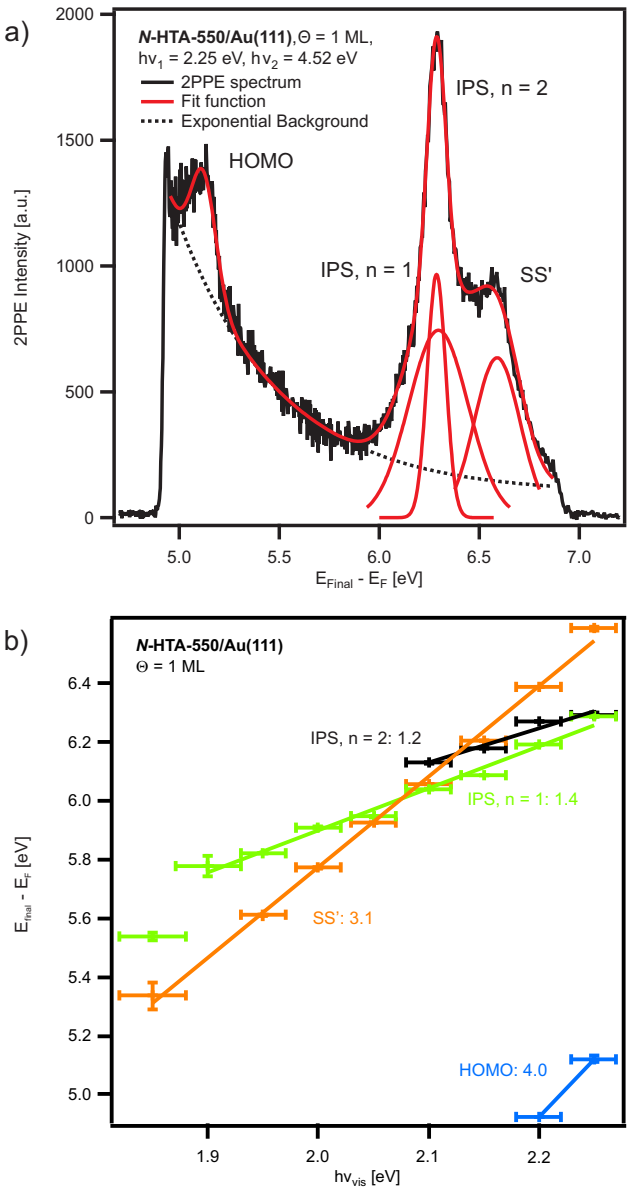

Figure S6: a) Two-color 2PPE spectrum of 1 ML *N*-HTA-550 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves; IPS: image potential state; SS: surface state). b) Photon-energy-dependent peak position extracted to assign peaks observed in the 2PPE spectrum to occupied and unoccupied intermediate electronic states. The slopes from the fits are given next to the respective data.

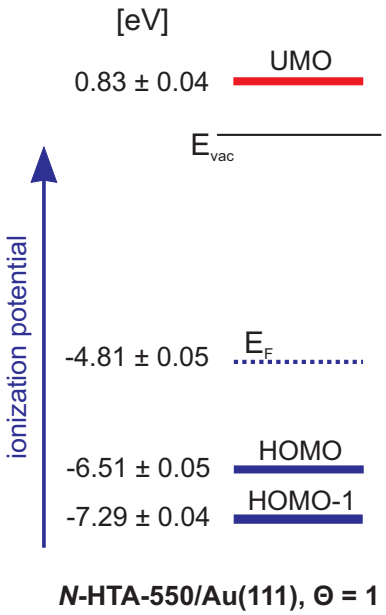

Figure S7: Energy level diagram of 1 ML *N*-HTA-550/Au(111) with respect to the vacuum level. The blue levels are the ionization potentials, which are in the molecular orbital picture represented by the energies of the HOMOs (UMO: unoccupied molecular orbital). E_F is the Au(111) Fermi level and E_{vac} is the vacuum level.

2 Two-photon photoemission data of *N*-HTA-557 adsorbed on Au(111)

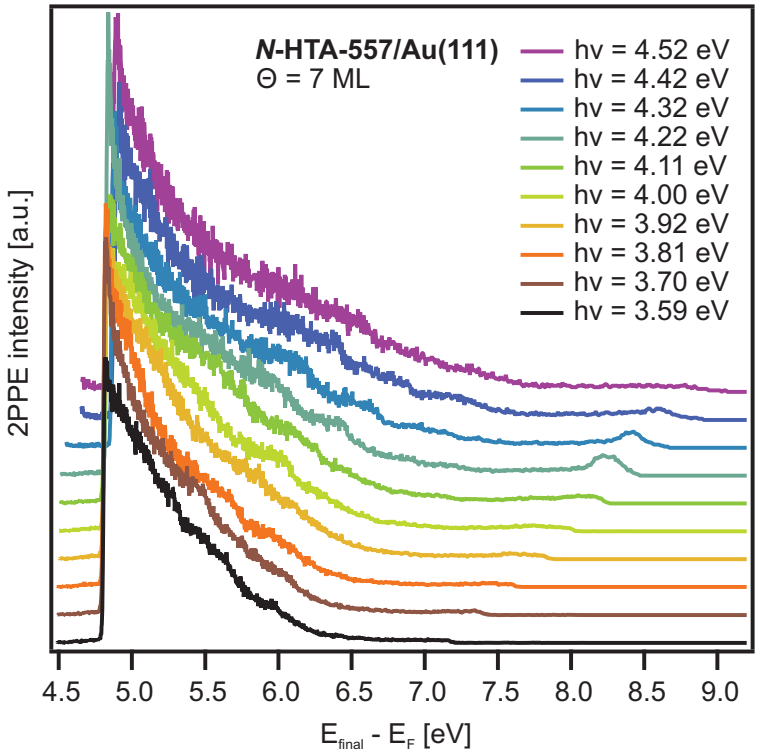

Figure S8: Photon energy dependent 2PPE spectra of 7 ML *N*-HTA-557 adsorbed on Au(111). The energy axis reveals the final state (E_{Final}) of photoemitted electrons with respect to the Fermi energy E_F ($E_{Final} - E_F = E_{kin} + \Phi$); thus, the low-energy cutoff corresponds to the work function (Φ) of the adsorbate/substrate system.

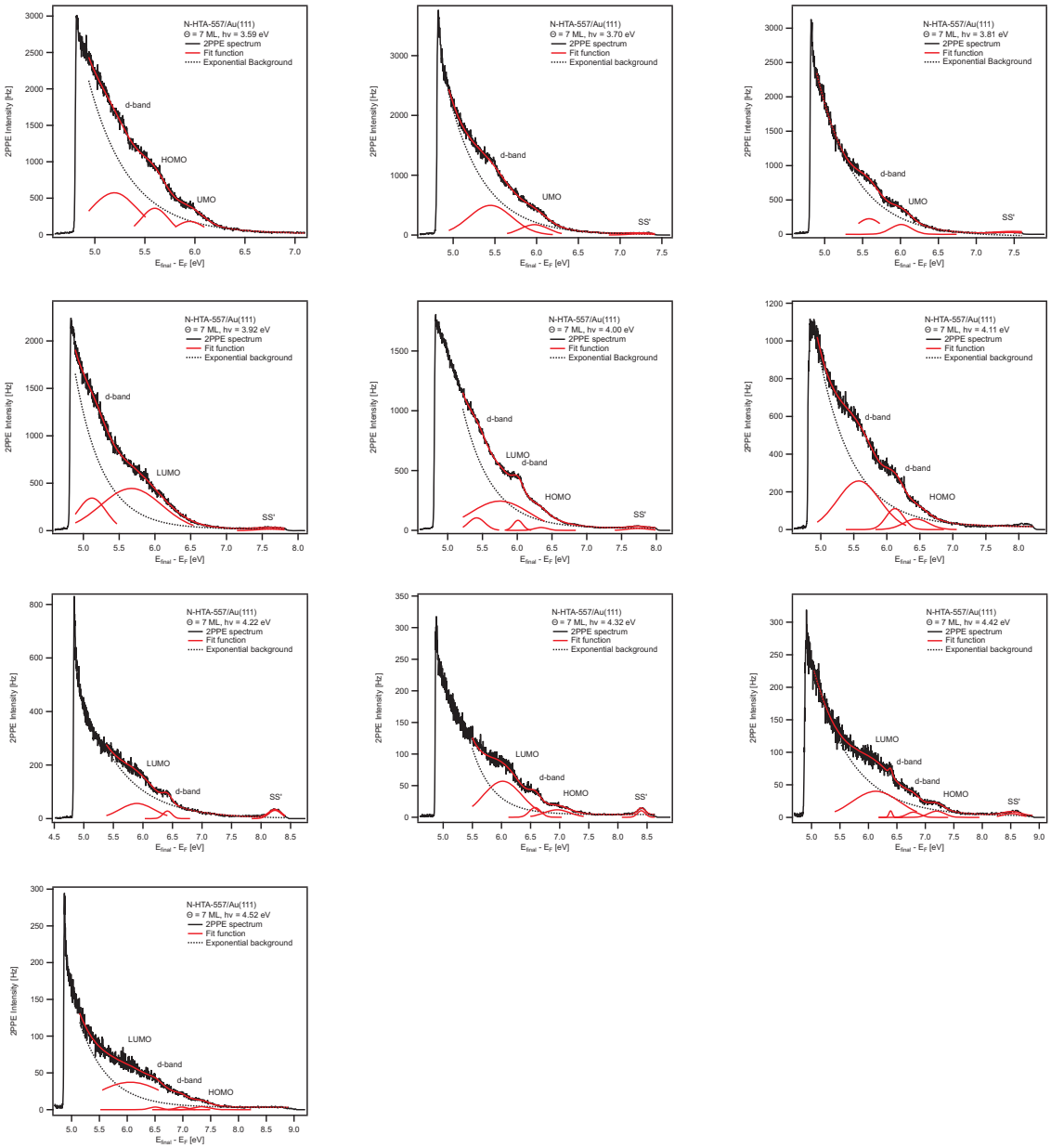

Figure S9: Photon energy dependent 2PPE spectra of 7 ML *N*-HTA-557 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves).

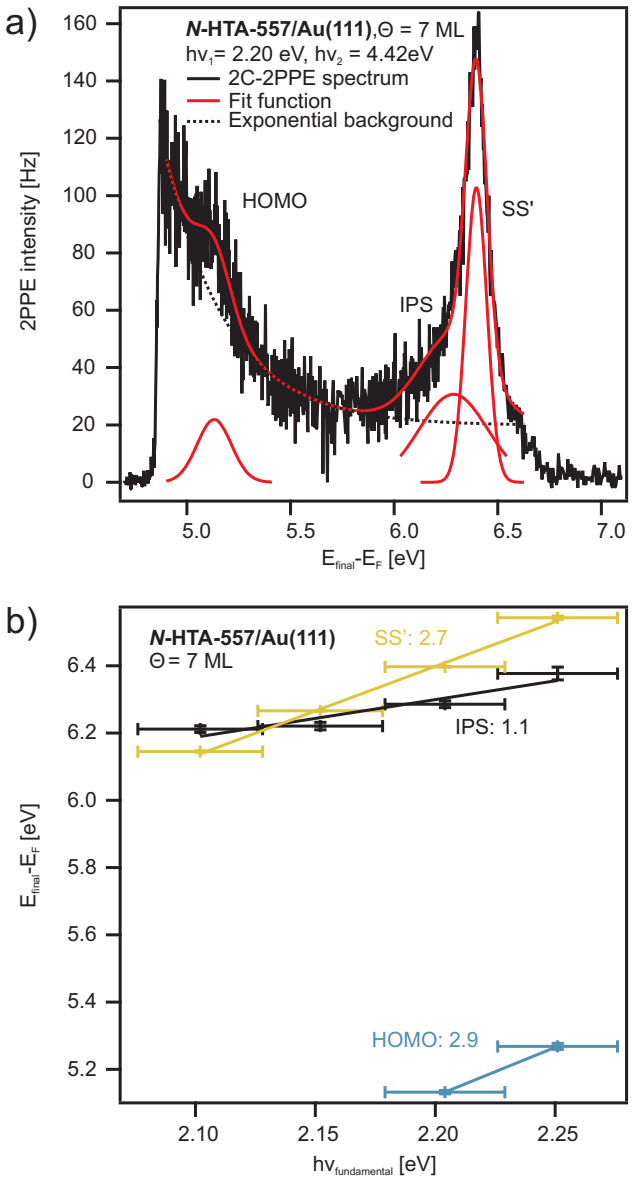

Figure S10: a) Two-color 2PPE spectrum of 7 ML ML *N*-HTA-557 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves; IPS: image potential state; SS: surface state). b) Photon-energy-dependent peak position extracted to assign peaks observed in the 2PPE spectrum to occupied and unoccupied intermediate electronic states. The slopes from the fits are given next to the respective data.

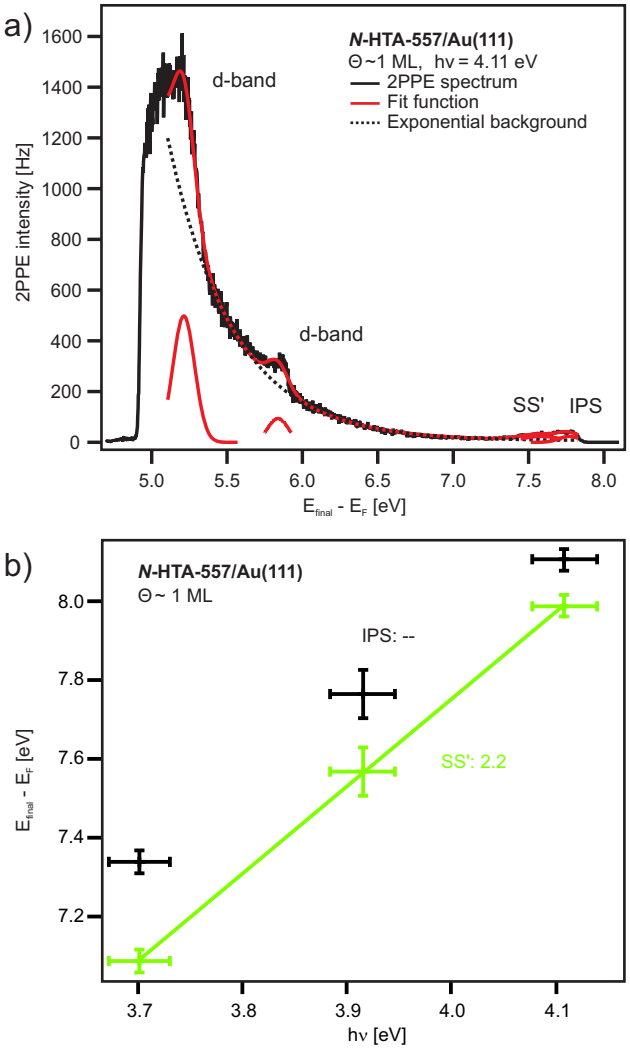

Figure S11: 2PPE spectrum of 1ML *N*-HTA-557 adsorbed on Au(111). The data are fitted with an exponential background and Gaussian-shaped peaks (red curves). b) Photon-energy-dependent peak position.