Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Dithiocarbamate anchoring group as flexible platform for interface engineering

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Computational details

Considered structures – Starting geometries and optimization procedure.

The starting geometry for PPz was chosen as follows. First, the isolated molecule was optimized in gas phase. With the distance between the two S atoms in the optimized structure comparable to the one between two high symmetry docking sites on the Au(111) surface, several trial geometries were set up, with the docking groups in fcc-hollow, hcp-hollow and on top positions, respectively. For all docking positions both a cofacial and a herringbone arrangement were tested. A preliminary geometry optimization was performed using the FHI-aims light default basis set. The most stable cofacial and herringbone arrangements were then further optimized using the tight default basis set. On these two geometries, the impact of twisting the phenyl rings by 90° was tested, too, to check the role of intra-molecular interactions. The final, optimized geometries of the four polymorphs are shown in Figure S1. The overall most stable arrangement is herringbone coplanar (see Table 2 in the main paper).

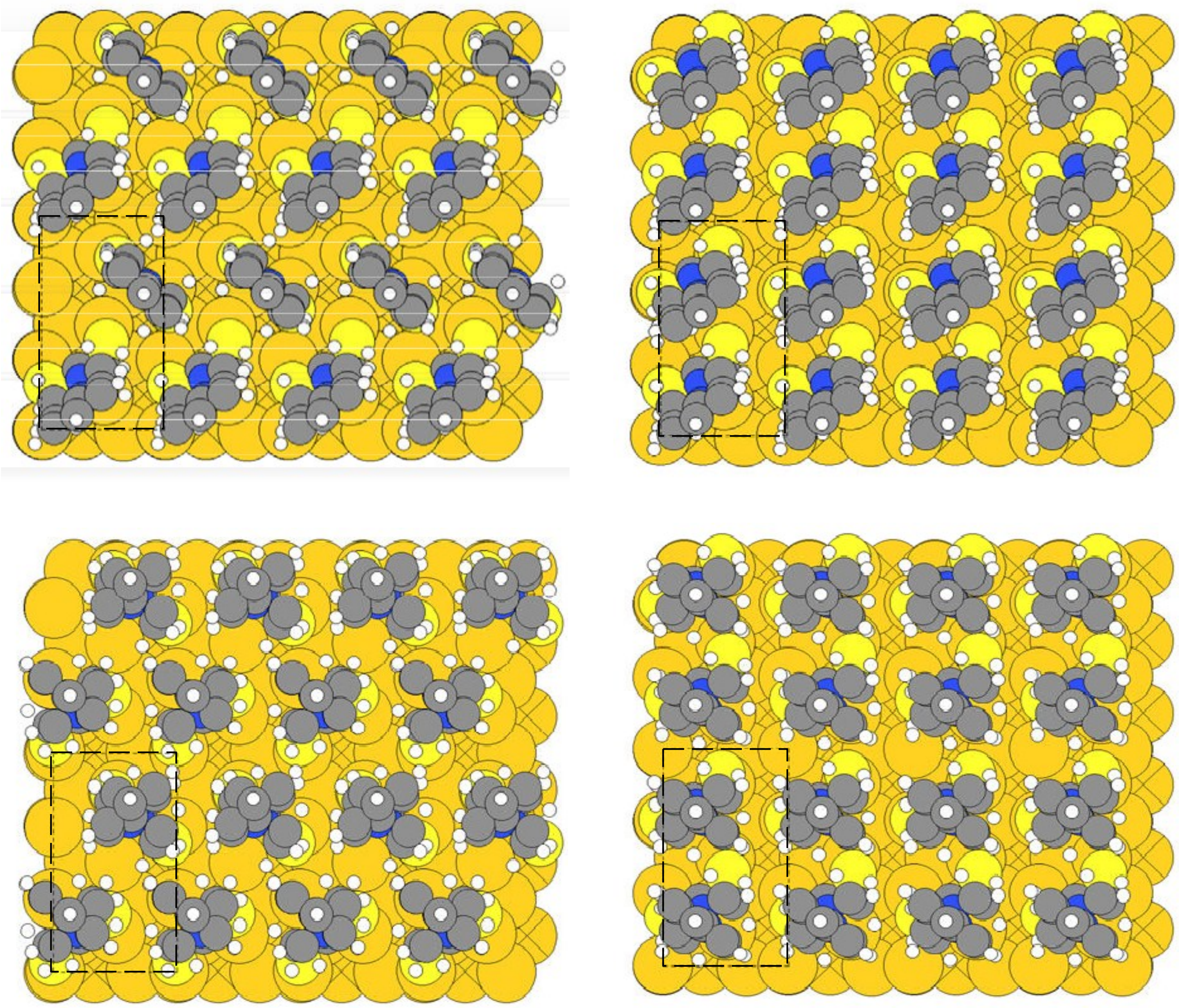

Figure S1. herringbone coplanar (top left panel), cofacial coplanar (top right panel), herringbone twisted (bottom left panel) and cofacial twisted (bottom right panel) optimized PPz geometries. The unit cell is marked by the dashed black line. Au atoms are depicted in dark yellow, S atoms in light yellow, C atoms in gray, N atoms in blue and H atoms in white.

Both in the herringbone and cofacial arrangements, the four S atoms in the unit cell occupy essentially the same docking positions: one docks in ontop position, one in bridge position and the remaining two dock in ontop positions shifted towards hollow/bridge sites (see Figure S2) in agreement with the experimentally observed inequivalent S docking positions (see main paper).

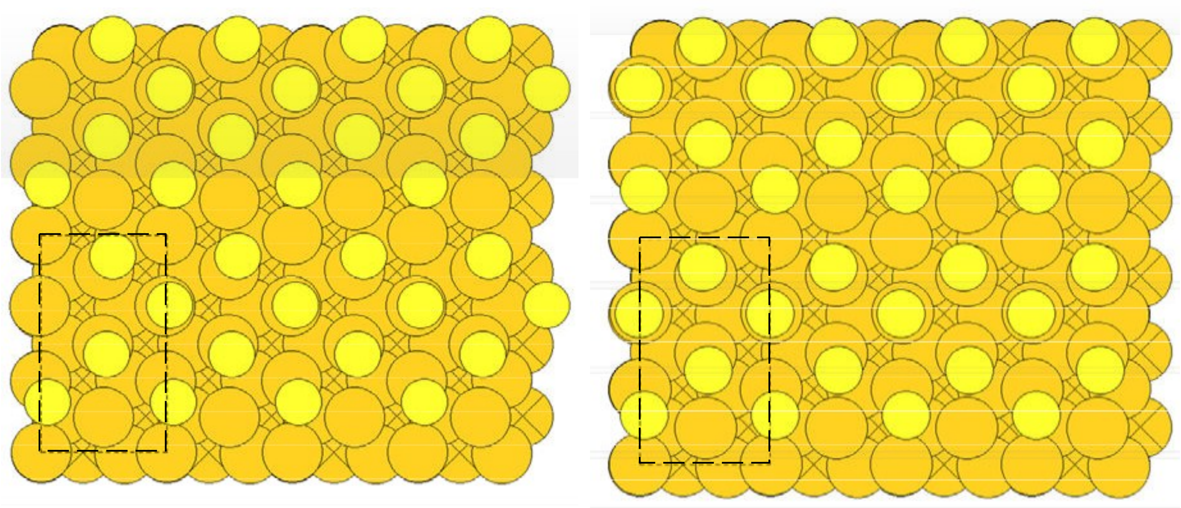

Figure S2. S positions in the herringbone (left) and cofacial (right) optimized geometries. The unit cell is marked by the dashed black line. Au atoms are depicted in dark yellow, S atoms in light yellow.

The above strategy to identify the most suitable arrangement and conformation performs a restricted sampling of the potential energy surface. There could in principle be (many) other ways for the molecules to dock to the surface and possibly larger unit cells containing a larger number of symmetry-inequivalent molecules. An extensive exploration of the full potential energy surface is beyond the purpose of the present work. Nevertheless, it is worthwhile to note that all the initial starting geometries (both cofacial and herringbone arranged) ended up with the S atoms occupying essentially the same sites. Moreover, it is interesting to take a look at the work function change ΔΦ for the different polymorphs (Table S1, where also the total energies are reported): within the same arrangement (cofacial or herringbone) the values are similar (with the exception of the least stable polymorph). A larger difference can be noted comparing cofacial and herringbone polymorphs, while between coplanar and twisted SAMs the difference is much more relevant (see Table 1 in the main paper).

Table S1: energy per unit cell and work function change (ΔΦ) of different coplanar PPz polymorphs, named after the arrangement (Hb for herringbone and Cf for cofacial) and the initial position of the docking atoms. The given values are slightly different from the ones reported in the main text due to the light basis set used for the preliminary optimizations. Only the most stable polymorphs for every arrangement (Hb hcp and Cf hcp) were subsequently optimized using the tight basis set.

Polymorph	**Energy per unit cell (eV)**	**ΔΦ (eV)**
Hb hcp	-16142284.468	-1.69
Hb fcc	-16142284.366	-1.64
Hb ontop	-16142284.426	-1.70
Cf hcp	-16142284.023	-1.51
Cf fcc	-16142283.971	-1.54
Cf ontop	-16142283.420	-1.63

For PPd, we first performed several tests on isolated, gas phase molecule, optimizing the geometries of different conformers. This was done to take in account that the piperidine ring can assume different conformations (chair, boat, twist, half chair) and that the H atom and the phenyl ring in position 4 can orient in different ways with respect to the lowest part of the molecule. Since these conformers are separated by energy barriers that are very unlikely overcome during the optimization, this approach was adopted to sample the potential energy surface, although to a limited extent. The most stable structure obtained this way was used to set up the unit cell. Considering that both the PPz and PPd molecules have the same bottom part, it is reasonable to assume that they will also have the same docking sites. Moreover, in the PPz case the impact of different starting S atoms arrangements turned out to have a negligible impact and all tested arrangements resulted in the same S atom positions. Based on this reasoning, the docking arrangement of the PPz optimized geometry was then used as starting point for building the PPd SAM: the metal part and the bottom part of the molecules were kept and the uppermost part was replaced, using the most stable conformer. The structures were subsequently optimized using the FHI-aims tight default basis set and are shown in Figure S3. Both, the herringbone and the cofacial arrangement and both the coplanar and the twisted conformation were tested, similar to what has been done for PPz. Again, as shown in the main text, the herringbone arrangement is more favourable, but contrary to PPz, in the most stable geometry the molecules assume a twisted conformation.

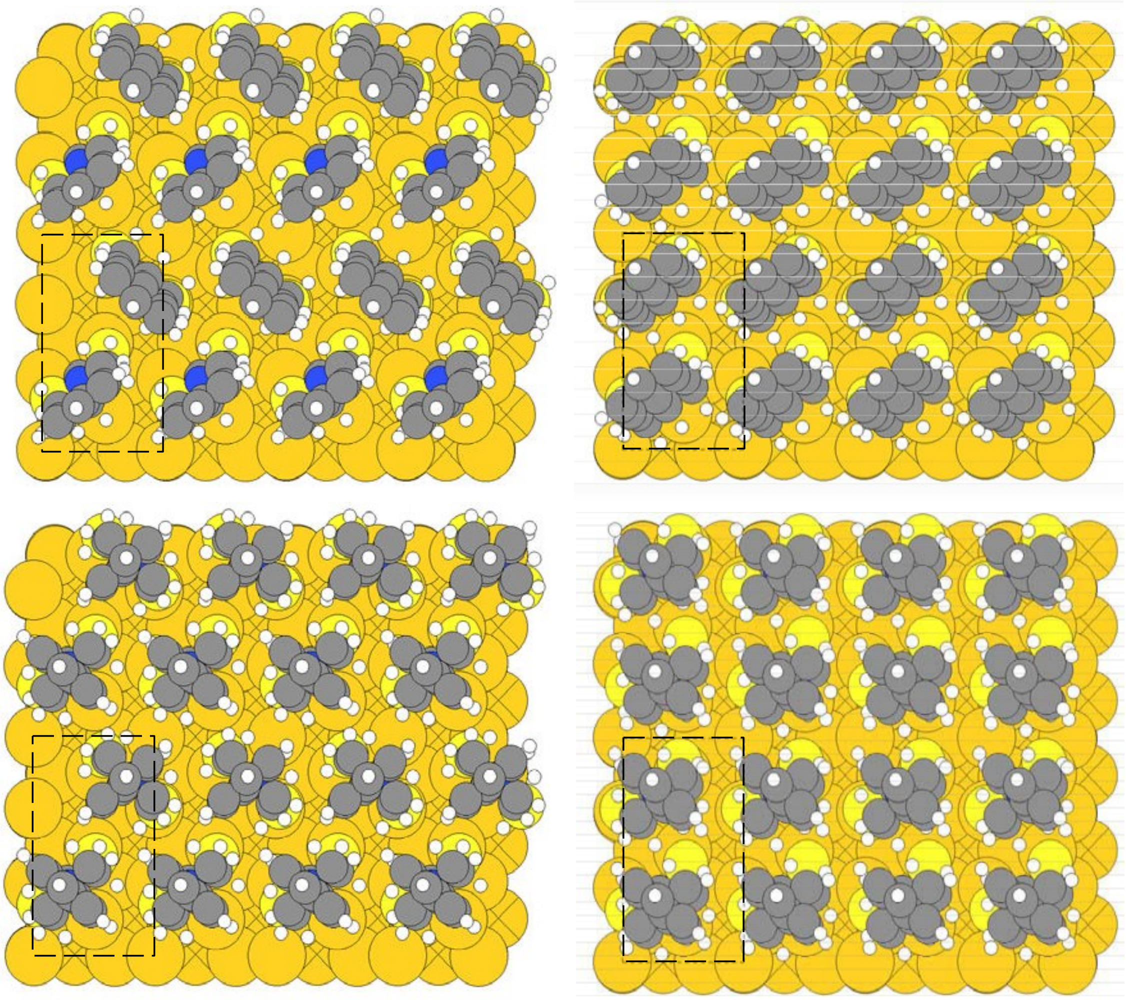

Figure S3. herringbone coplanar (top left panel), cofacial coplanar (top right panel), herringbone twisted (bottom left panel) and cofacial twisted (bottom right panel) optimized PPd geometries. The unit cell is marked by the dashed black line. Au atoms are depicted in dark yellow, S atoms in light yellow, C atoms in gray, N atoms in blue and H atoms in white.

With the C atom in position 4 in the piperadine ring sp^3 hybridized, in the PPd herringbone SAM there could in principle be four different ways for the molecules to arrange with respect to the neighbours. This is due to the different orientations of the phenyl ring and the H atom bonded to that C atom. To see how this would possibly impact the observables, an optimization using a light basis set was performed. The optimized structures are shown in Figures S4 and S5, where also the names assigned to them are given.

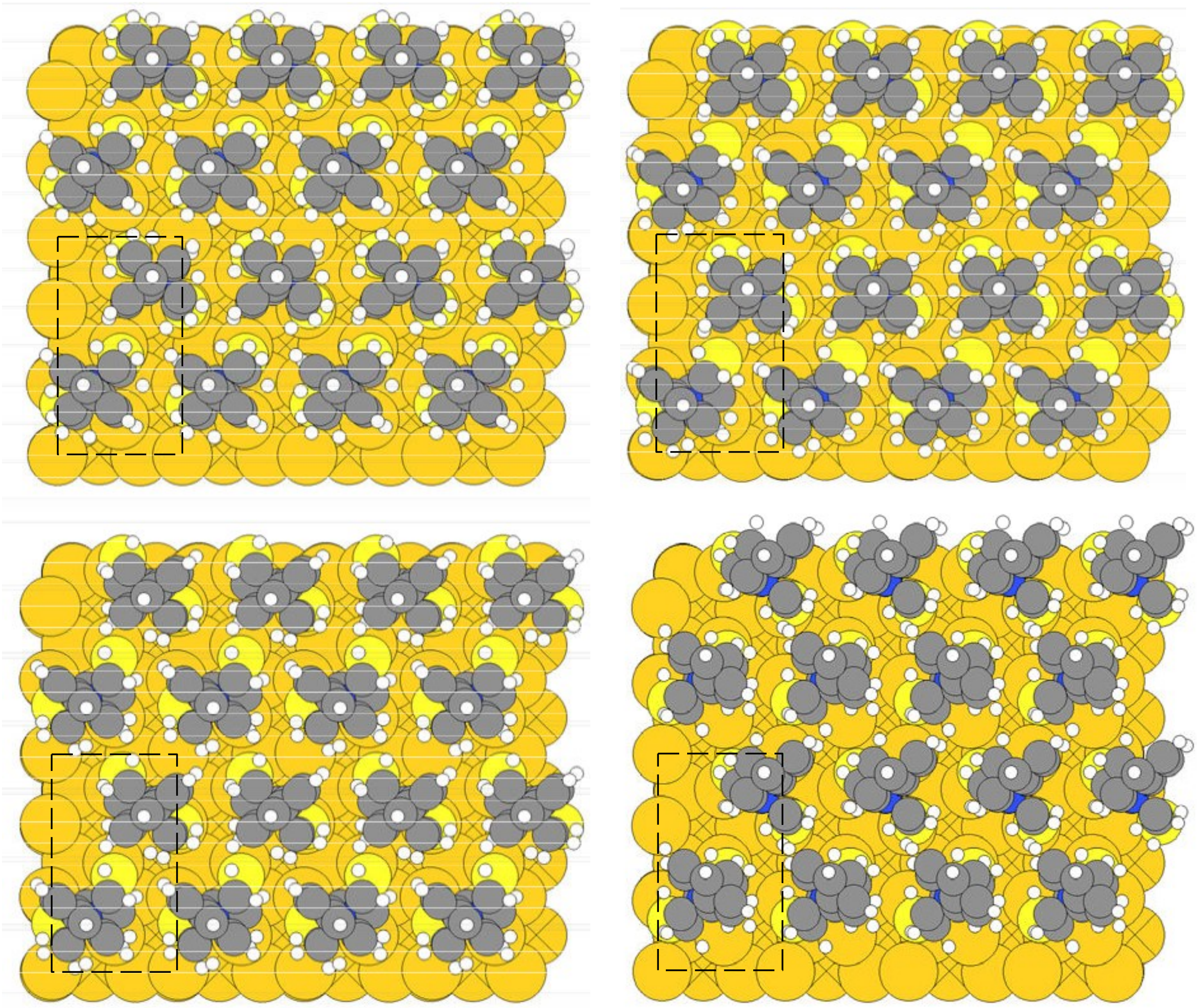

Figure S4. four different PPd herringbone twisted conformers. Top left: tw1 (most stable conformer), top right: tw2, bottom left: tw3, bottom right tw4.

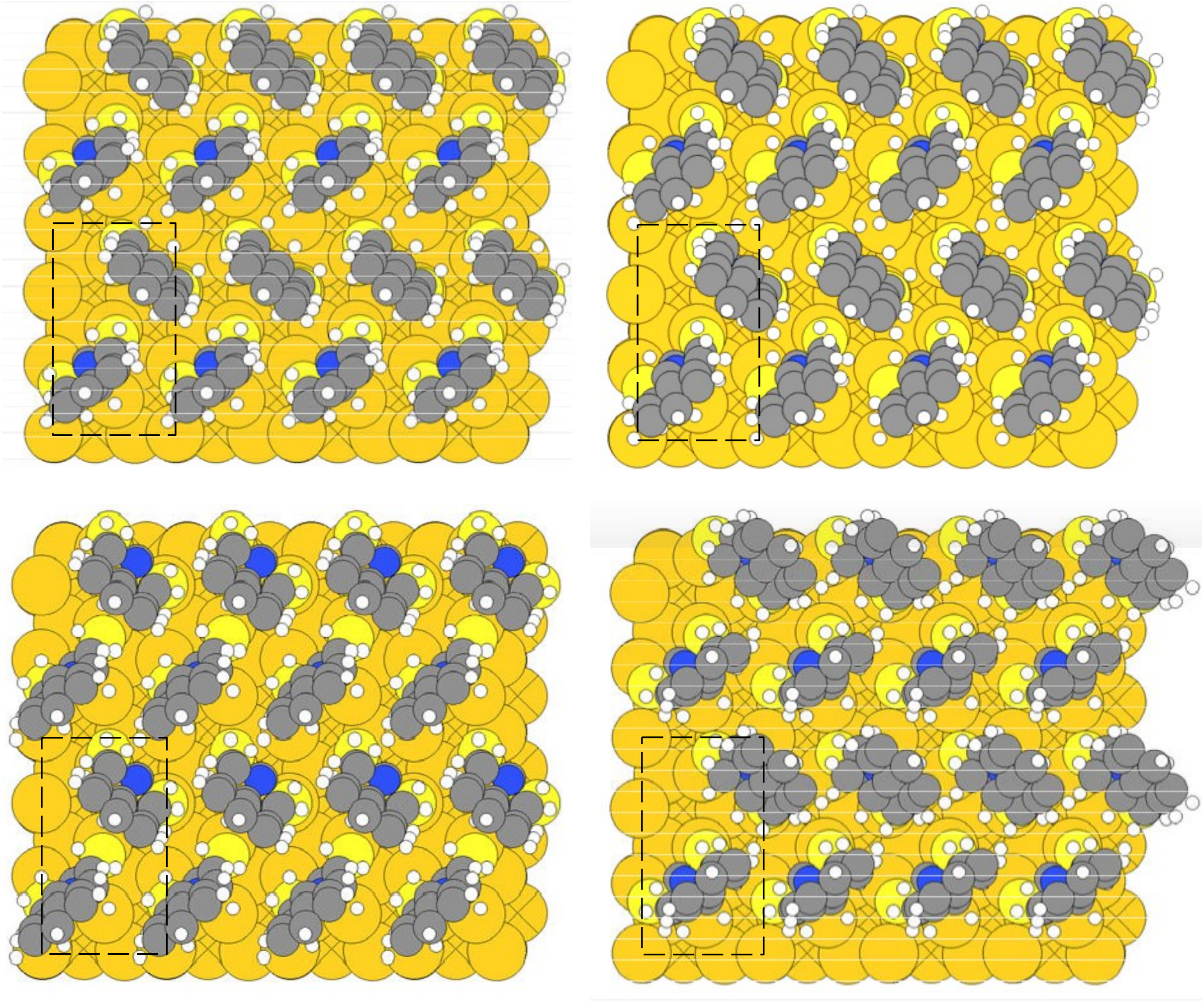

Figure S5. four different PPd herringbone coplanar conformers. Top left: cf1 (most stable conformer), top right: cf2, bottom left: cf3, bottom right cf4.

The energy and work function change values are reported in Table S2. A certain variability in the work function change can be noticed, with on average larger values for the twisted polymorphs. However, no clear trend can be identified. The conformers named 1cp and 1tw are the most stable among the coplanar and the twisted ones, respectively, and were used for the optimization with the tight basis set.

Table S2: energy per unit cell and work function change (ΔΦ) of the different herringbone twisted and coplanar PPd conformers. All values are given relative to the most stable structure (1tw). The structures are named according to figures S4 and S5. The given values are slightly different from the ones reported in the main text due to the light basis set used for the preliminary optimizations. Only the most stable twisted and coplanar conformers (1tw and 1cp) were subsequently optimized using the tight basis set.

Polymorph	**Energy per unit cell (eV)**	**ΔΦ (eV)**
1tw	0.00	-2.59
2tw	0.10	-2.51
3tw	0.35	-2.46
4tw	0.19	-2.56
1cp	0.11	-2.53
2cp	0.28	-2.35
3cp	0.14	-2.54
4cp	0.53	-2.45

Tilt angles of the π* orbitals of the phenyl ring and molecular tilt and twist angles of the main conformers

The calculated tilt angles of the π* orbitals of the phenyl ring (α) and the molecular tilt and twist angles (β and γ, respectively) for the main conformers of the PPz and PPd SAMs are reported in table S3. The values of the two inequivalent molecules in the unit cell are given. Additionally, the average value of α is reported calculated as defined in the caption of Table 3 in the main text. Since the phenyl C atoms are not all perfectly in a plane, the choice of the atoms used to define the plane of the ring could slightly change the obtained value. The differences were, however, found to be negligible and for sake of consistency for every polymorph the plane of the phenyl ring was defined by taking the atoms in position 1 and 4 together with the next atom with the lowest z coordinate

Table S3: calculated tilt angles of the π* orbitals of the phenyl ring and molecular tilt and twist angles of the main PPz and PPd conformers. The subscripts 1 and 2 refer to the two inequivalent molecules in the unit cell. Additionally, for α the average value according to the equation given in the caption of Table 3 in the main paper is given.

			α (°)			β (°)		γ (°)	
			α_1	α_2	α_{av}	β_1	β_2	γ_1	γ_2
PPz	herringbone	coplanar	84.1	79.0	81.2	7.4	13.7	37.6	36.1
		twisted	89.5	81.0	83.6	0.7	10.6	44.3	31.4
	cofacial	coplanar	82.5	81.6	82.0	11.0	9.8	47.0	30.6
		twisted	89.3	88.9	89.1	4.9	4.2	81.9	74.4
PPd	herringbone	coplanar	89.6	77.5	81.2	6.2	12.9	86.5	14.2
		twisted	82.5	80.6	81.5	14.2	12.6	58.0	41.1
	cofacial	coplanar	72.8	73.3	73.0	17.8	16.8	13.9	6.0
		twisted	86.1	85.0	85.5	10.9	12.1	68.8	65.2

Details of the employed computational methods

The preliminary geometry optimizations mentioned in the previous section were performed setting the following self consistency cycle criteria: sc_accuracy_rho 1e-5, sc_accuracy_etot 1e-

6, sc_accuracy_forces 1e-4, sc_accuracy_eev 1e-3. The C and N atoms were described using a "Tier 1" basis consisting of the minimal basis plus one set of basis functions up to d-functions. The H atoms were described using a "Tier 1" basis consisting of a minimal basis plus one set of basis functions up to p-functions. The S atoms were described using the minimal basis plus the s-, p- and d-functions of the "Tier 1" set of basis functions. The Au atoms were described using a "Tier 1" basis, consisting of the minimal basis plus one set of basis functions up to h-functions. The cutoff potential of all basis functions was set to 3.5 Å.

The more accurate geometry optimizations were performed using basis set described in the main paper and adding the self consistency cycle accuracy criterion sc_accuracy_potjump 1e-4 (see control.in file included below). Regarding the reduced coverage unit cells, 1/16 and 1/36 coverage were considered. Since calculating them using the previously described settings would have been computationally particularly expensive, as already mentioned in the main text the metal bulk was modelled with 3 layers of Au instead of 5 and the following reduced settings for basis set and self-consistency criteria were applied: The tags sc_sccuracy_rho and sc_accuracy_etot were set to 1e-3 and 1e-4, respectively. The sum of eigenvalues (sc_accuracy_eev) and the vacuum level potential shift (sc_accuracy_potjump) were not used as convergence criteria. For the C, H, N and S atoms the basis set described in the main paper and reported below was used. For the Au atoms the basis was modified as follows: the l_hartree tag was set to 4, the onset radius of the cutoff potential to 3.9 and the radial width of the cutoff potential to 1.8, one more division line was commented, the outer grid was consequently set to 302 and the h basis function of the first tier was commented. These settings were chosen according to the convergence test explained below.

The calculations on the periodic systems and on the isolated gas phase molecules were performed defining the occupation of the Kohn – Sham eigenstates using a Gaussian broadening function and setting the width to 0.1 and 0.01 eV, respectively.. The core level energies were obtained from the atom projected density of states output files (2001 data points for a range of 20 eV with the value for the Gaussian broadening set to 0.1 eV). The energy (first column of the output file) corresponding to the maximum value of the total dos (second column of the output file) was taken as the value of the core level binding energy. The energy ranges were chosen after calculating the core level energies of a single isolated atom.

The aforementioned convergence tests were performed to guarantee that the use of reduced and less expensive computational settings still gives reliable and converged results. Convergence is reached when the results obtained using more accurate settings differ by less than a certain convergence criterion, set according to the purpose of the calculation. The value of the work function change and of the relative core level energies were taken as convergence criteria. Regarding the basis set, for the investigated cases the results obtained using the FHI-aims default tight settings were compared to the ones obtained increasing the accuracy of the settings: for every element the onset radius and the radial width of the cutoff potential were increased to 4.1 and 2.1 Å, respectively, the radius of the outermost shell of the basic grid was increased to 7.1 Å, the radial multiplier was set to 3, the outer_grid tag was set to 590, the corresponding division line of the angular_grids tag was uncommented and a further basis function was added, specifically the first basis function of the second tier for Au, the first of the third tier for H, C and N and the third of the second tier for S. Regarding the k-points, the 5x9x1 k-point grid was compared to a 15x27x1 grid. The variations in the work-function modification were always below 0.025 eV and the relative core level energy differences always below 0.010 eV, values widely acceptable for the present purposes.

The Au bulk was modelled using the theoretically optimized lattice constant value. To obtain that, single point calculations were performed using different lattice constants, the total energy was plotted as a function of the lattice constant and the curve was fitted with a quadratic function. The value of the lattice constant corresponding to the minimum of the curve was taken as the optimized one. The value of the lattice constant was changed by 0.0025 Å each step. A conventional unit cell with 4 Au atoms was used. A 12x12x12 and a 24x24x24 k-points grid were adopted, with the obtained values being in agreement up to the third decimal digit. The obtained value for the lattice constant was 4.158 Å, corresponding to a nearest neighbour distance of 2.940 Å. The same settings adopted to get the optimized lattice constant were employed to describe the Au atoms in any calculation used to get the reported results.

Calculation of the work function change

The work function change has been calculated as the difference between the work function of the SAM/Au(111) systems and the work function of a clean Au(111) slab. The same settings were used for the optimization and in both cases the three bottom Au layers have been kept fixed during all the calculations while the topmost two have been relaxed.

Details of the XP spectra simulations

The damping factor for weighting the contribution of every atom was introduced using the following exponential attenuation function:

$$w_i(d) = w_0 \exp\left(-\frac{d}{\lambda}\right).$$

w_0 is a scaling constant that does not change the shape of the spectrum. $w_i(d)$ is the individual weigth of the i-th atom, that depends on the vertical distance d between the atom and the topmost C atom in the SAM and on a damping factor λ. According to Lamont and Wilkes,[1] λ is defined as $\lambda=0.3E_{kin}^{\beta}$, where E_{kin} is the kinetic energy of the escaping electron and β is an empirical attenuation factor. E_{kin} is given by the difference between the energy of the incident photon (350 eV in this case) and the calculated binding energy of the C 1s electron. The value of β was set to 0.405, after tuning it in such a way that the calculated relative intensities of the peaks matched the experimental ones.

Further information on the calculated core-level binding energies

Estimate of the impact of the reduced coverage measured for the PPd SAM on its electrostatic properties:

To estimate the impact of reduced coverage and ensuing disorder in the PPd SAMs on the SAM-induced shift in electrostatic energy, ΔE, one can start from the ideal situation considered in the simulations and then estimate the impact of reduced coverage,Θ, and increased molecular tilt, β, observed in the experiments via:

$$\Delta E^{*} = \Delta E \cdot \frac{\cos(\beta_{calc})\,\Theta_{calc}}{\cos(\beta_{exp})\,\Theta_{exp}}$$

Inserting the values from Tables 1, 2, and 3 of the main manuscript (for the latter taking the average of the two molecules in the unit cell) and setting Θ_{calc} to 1, one obtains:

Δ⍰* ൧ ൗΔE ൧൧ 0.90

Based on the calculated shift in electrostatic energy, which corresponds to the work-function change ($\Delta\Phi_{PPd,calc}$ =2.54) this yields ΔE*= 2.29 eV (i.e., a disorder-induced reduction by 0.25 eV). Note that the above considerations only provide a rough estimate, as they neglect the coverage dependence of depolarization effects, for the experimental tilt-angle only the lower boundary can considered, and also a possible tilt-angle dependence of the interfacial charge transfer is neglected.

Inequivalent molecules in the full coverage unit cell

As already explained in the main text, in the full coverage unit cell used in the simulations there are two molecules. Since they are not symmetry equivalent and have slightly different tilt angles, there are some small differences also in the core level energies. In figure S6 a (PPz) and b (PPd) the non screened energies of the two molecules in the full coverage unit cell of the most stable polymorph are reported. The energies are given without any shift and screening effects are not included either, as we are seeking for “conceptual” differences between the core-level binding energies of the C atoms, which would just be obscured by a distance-dependent screening. In the simulation of the full coverage XP spectrum the average values were taken in account. Since for the reduced coverage case only one molecule was kept in the unit cell, the comparison was always made taking as reference the molecule of the full coverage case used to set up the low coverage unit cell.

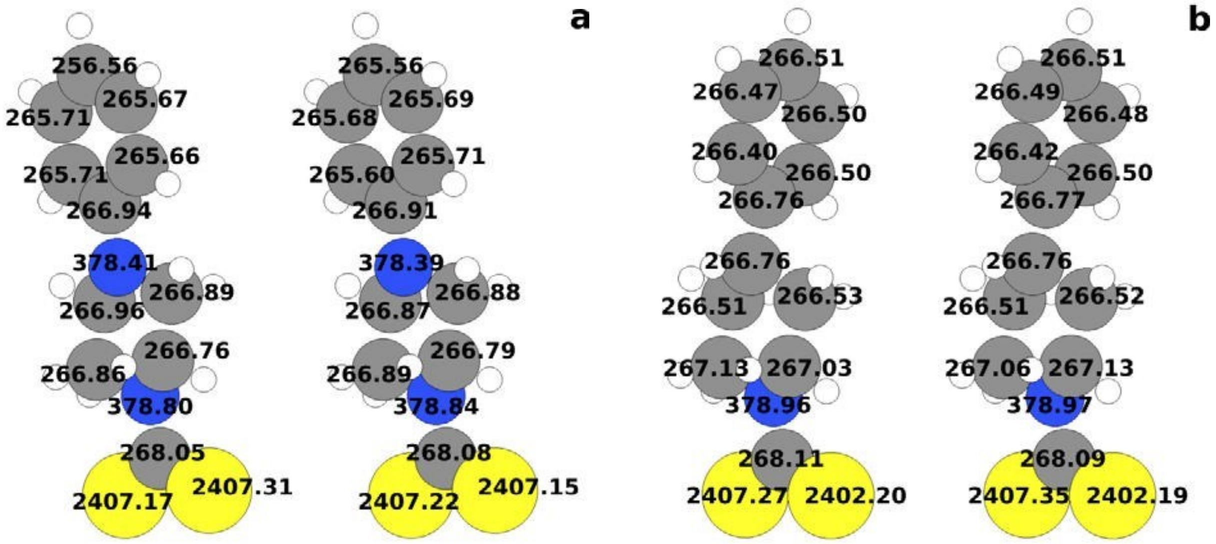

Figure S6. C 1s core level energies without screening effects of the PPz (a) and PPd (b) molecules in the full coverage unit cell. Carbon atoms are depicted in grey, H in white, N in blue and S in light yellow.

PPz binding energies

As reported in the main text, the 1s binding energy of the topmost C atoms is shifted relative to its neighbors both at full and at reduced coverage. To understand that shift, the C 1s core level binding energies were calculated for the isolated PPz molecule, this way excluding any non chemical effects. From the energy values, reported in figure S7, one can see that the shift of about 0.2 eV between the topmost C atom and its neighbours is still present.

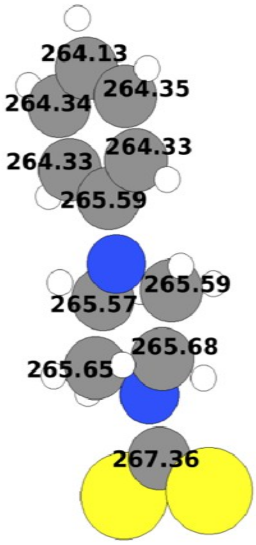

Figure S7. C 1s core level energies of an isolated PPz molecule. Carbon atoms are depicted in grey, H in white, N in blue and S in light yellow.

The chemical origin of this shift can be better understood considering the aniline molecule as model system (figure S8). In this case the difference between the carbon in position 4 and the carbons in positions 3 and 5 is larger and a shift is also present between these 2 latter carbons and the ones in position 2 and 6, whereas in the PPz molecule this is not the case. Looking at the resonance forms of aniline (figure S9), a negative charge is sitting on the ortho and para positions, consistent with a smaller absolute values of the core level energies of these atoms with respect to the other ones.

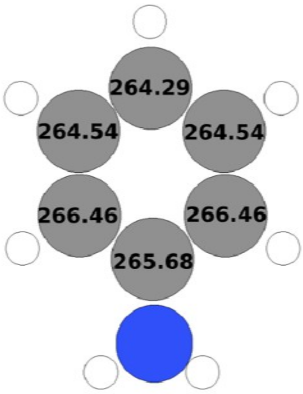

Figure S8. Calculated C 1s core level energies of aniline. Carbon atoms are depicted in grey, H in white and N in blue.

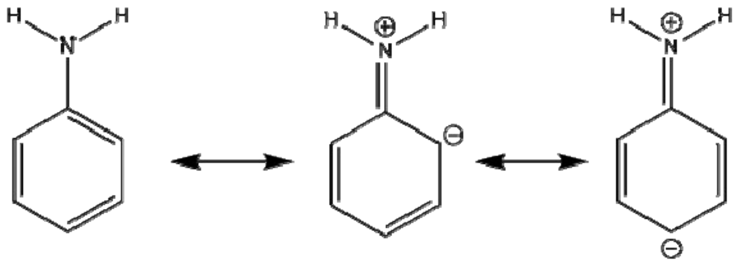

Figure S9. Resonance forms of aniline.

The difference between the para and the meta positions is larger than the one between the meta and the ortho ones: the ortho carbons bonded to the C1 feel the negative charge to a lower extent, because of the inductive effect due to the N atom. Comparing the aniline to the ph-piperazine-DTC, in the latter case the shifts are smaller (actually there is almost no difference between the meta carbons and the ortho ones). This can be understood considering that for ph-piperazine-DTC the nitrogen atom belongs to a piperazine ring instead of being bonded to two H atoms. Therefore, the negative charge that can delocalize is significantly smaller than in the aniline case.

Coverage-dependent shifts

In figures S10 a (PPz) and b (PPd) the C 1s, N 1s and S 1s core level energy differences between full and 1/36 coverage cases are given. It can be seen that the differences are larger for the atoms that are further away from the metal surface, meaning that the atoms closer to the surface to some extent feel the dipole also in the reduced coverage cases and that the effects of such a dipole rapidly decays moving away from it. The energy of the S atoms and of the C directly bonded to them show a very weak coverage dependence. In the PPd case the shift is larger, which is consistent with this system inducing a stronger interface dipole. This can be concluded also comparing the calculated work function changes: -1.71 eV for PPz and -2.58 for PPd.

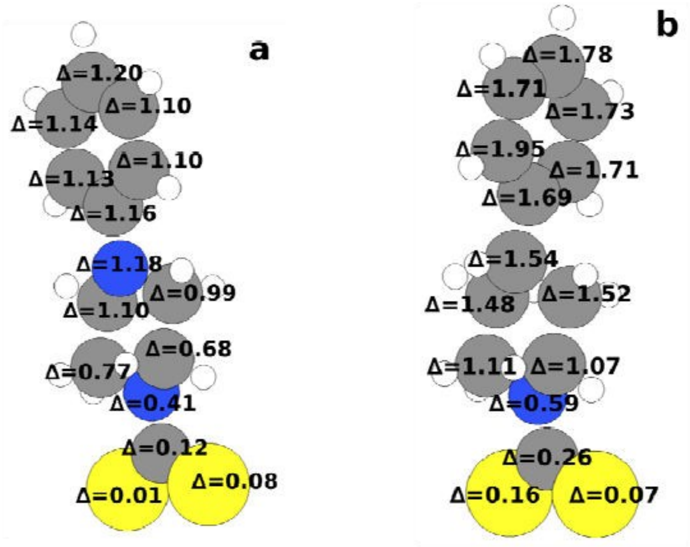

Figure S10. C 1s, N 1s and S 1s core level energy differences between full and 1/36 coverage for PPz (a) and PPd (b). C atoms are depicted in grey, H in white, N in blue and S in light yellow.

Coverage-dependent charge rearrangements and chemical core-level shifts

As mentioned in the main manuscript, one of the reasons, why the analysis of core-level shifts for atoms very close to the substrate becomes difficult is that the interfacial charge transfer and, correspondingly, the resulting chemical shifts in core-level binding energies vary with coverage.

To illustrate that, we analyze the (plane integrated) charge rearrangement per molecule, Δρ, due to the bonding of PPz to the Au substrate. Such rearrangements are modeled via the following equation:

$$\Delta\rho = \frac{1}{n}\rho_{SAM/Au} - \left(\rho_{Au} + \rho_{SAMH} - \rho_{H}\right)$$

where n is the number of molecules in the unit cell and Δρ is calculated using the charge densities associated with the combined SAM/metal system, $\rho_{SAM/Au}$, the isolated metal slab, ρ_{Au}, the isolated SAM with the S atoms saturated with H atoms, ρ_{SAMH}, and the isolated H atoms, ρ_{H}. To get the charge densities of the subsystems, the geometries they later adopt in the optimized combined structure were maintained. In the SAMH case, only the position of the H atoms was relaxed. The optimized H positions were then used to calculate ρ_{H}. For the plot, the quantity Δρ was integrated over the xy plane within the unit cell. Δρ for the full and reduce coverage case of the PPz SAM are plotted in figure S11.

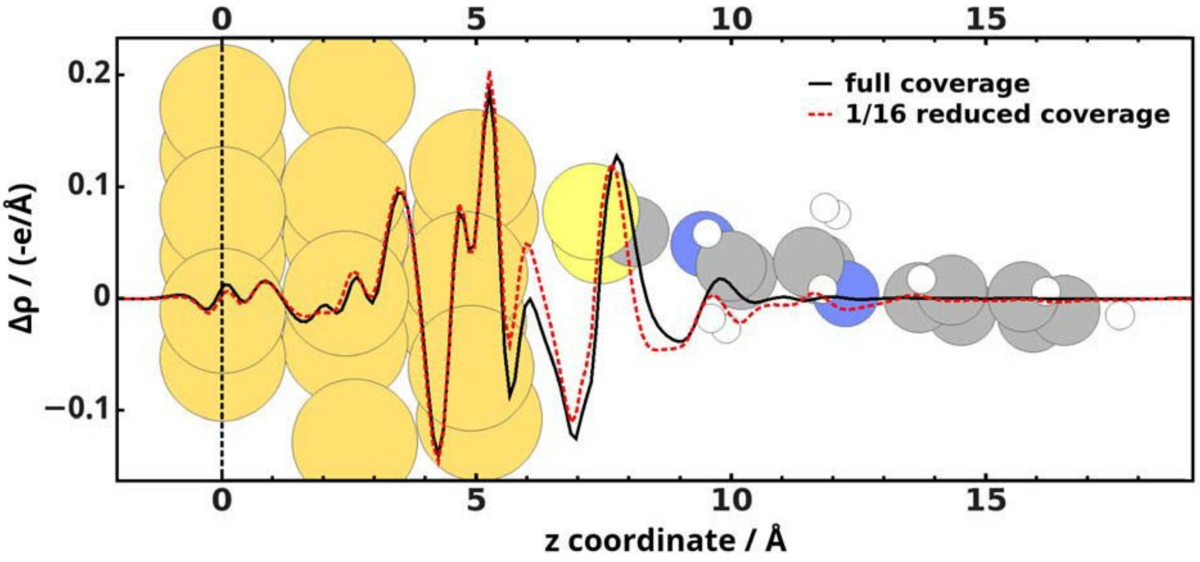

Figure S11. xy-plane integrated Δρ per molecule for the full (black solid line) and 1/16 reduced (red dashed line) coverage case of the PPz SAM.

Of particular relevance in the present context is the difference in Δρ between full and 1/16 coverage, which is shown in Figure S12. It reveals opposing coverage dependences of the charge rearrangements at the z-positions of the S atoms and the adjacent C atom.

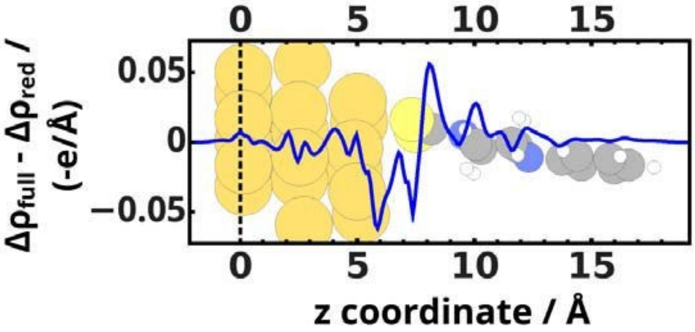

Figure S12. Difference between the z-dependent charge rearrangement per molecule integrated over the (xy)-plane within the unit cell in the full ($\Delta\rho_{full}$) coverage and in the 1/16 ($\Delta\rho_{red}$) reduced coverage cases for the PPz SAM.

Albeit small, such differences in charge rearrangements can results in chemical core-level shifts of several hundred meV, masking the impact of the local electrostatic potential for nuclei in the immediate vicinity of the interface. The magnitude of these coverage-dependent chemical shifts are estimated for the example of the C 1s core level energies of an isolated C atom in Figure S13. Charges between -e and e are considered and the energy values are referenced to the binding energy of the neutral atom. One can see that even small changes in the charge cause large shifts in the binding energy. Moreover, the more positive the charge, the larger the magnitude of the shifts. The obtained evolution is not strictly linear. As a consequence, the calculated slopes vary between 0.09 eV and 0.17 eV for the change in binding energy per 0.01×e change in atomic charge.

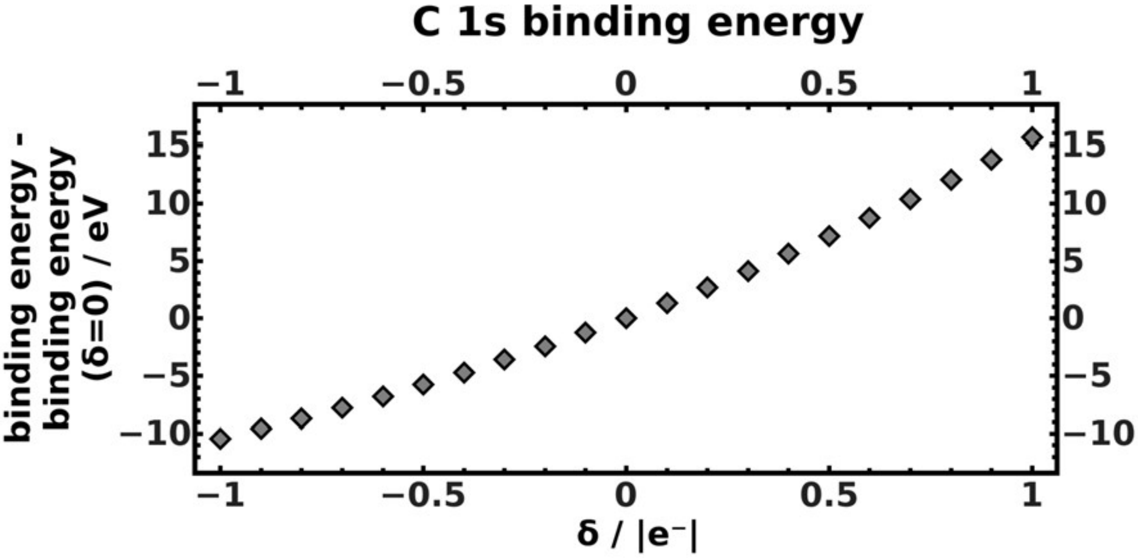

Figure S13. Evolution of the C 1s core level energies depending on the charge δ sitting on the C atom. The energies are given aligned to the 1s core level energy of the neutral C atom.

The simple model of charging a spherically symmetric atom cannot be quantitatively transferred to the much more complex charge rearrangement pattern at the DTC/Au(111) interface, but it shows that changes in the atomic charge of a few hundredths of the elementary charge (as observed in Figure 8 of the main manuscript) can result in BE shifts of several hundred meV.

APPENDIX

input file (control.in) containing the basis set used for the accurate geometry optimizations.

For the sake of reproducibility and for an unambiguous specification of the employed basis sets, in the following a prototypical FHI-aims input file is reproduced.

```
xc pbe
vdw_correction_hirshfeld
vdw_pair_ignore Au Au
compensate_multipole_errors .true.

mixer pulay
charge_mix_param 0.1
preconditioner kerker 1.1

charge 0
spin none
sc_accuracy_rho 1e-5
sc_accuracy_etot 1e-6
sc_accuracy_forces 1e-4
sc_accuracy_eev 1e-3
sc_accuracy_potjump 1e-04
relax_geometry trm 1e-2
occupation_type gaussian 0.1
relativistic atomic_zora scalar
k_grid 9 5 1
use_dipole_correction
evaluate_work_function

 species        Au
#     global species definitions
    nucleus             79
    mass                196.966569
    hirshfeld_param     134 15.6 2.91
#
    l_hartree           6
#
    cut_pot             4.0  2.0  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         73 7.0
    radial_multiplier   2
    angular_grids specified
      division   0.3416   50
      division   0.7206  110
```

```
      division   1.1171  194
      division   1.2821  302
      division   1.5560  434
      outer_grid  434
#############################################################
#
#  Definition of "minimal" basis
#
#############################################################
#     valence basis states
    valence      6  s   1.
    valence      5  p   6.
    valence      5  d  10.
    valence      4  f  14.
#     ion occupancy
    ion_occ     6  s   0.
    ion_occ     5  p   6.
    ion_occ     5  d   9.
    ion_occ     4  f   14.
#############################################################
#
#     Suggested additional basis functions. For production
calculations,
#   uncomment them one after another (the most important basis
functions are
#  listed first).
#
#  Constructed for dimers: 2.10, 2.45, 3.00, 4.00 AA
#
##############################################################
#  "First tier" - max. impr. -161.60  meV, min. impr. -4.53 meV
     ionic 6 p auto
     hydro 4 f 7.4
     ionic 6 s auto
     hydro 5 g 10
     hydro 6 h 12.8
     hydro 3 d 2.5
##############################################################
#
#  FHI-aims code project
# Volker Blum, Fritz Haber Institute Berlin, 2009
#
#   Suggested "tight" defaults for H atom (to be pasted into
control.in file)
#
##############################################################
  species        H
```

```
#     global species definitions
    nucleus             1
    mass                1.00794
#
    l_hartree           6
#
    cut_pot             4.0  2.0  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         24 7.0
    radial_multiplier   2
    angular_grids       specified
      division   0.1930   50
      division   0.3175  110
      division   0.4293  194
      division   0.5066  302
      division   0.5626  434
#      division   0.5922  590
#      division   0.6227  974
#      division   0.6868 1202
#      outer_grid  770
      outer grid  434
#######################################################################
#
#  Definition of "minimal" basis
#
#######################################################################
#     valence basis states
    valence      1  s
    1.
#     ion occupancy ion_occ
      1          s  0.5
#######################################################################
#
#     Suggested additional basis functions. For production
calculations,
#   uncomment them one after another (the most important basis
functions are
#  listed first).
#
#  Basis constructed for dimers: 0.5 A, 0.7 A, 1.0 A, 1.5 A, 2.5
A
#
#######################################################################
#  "First tier" - improvements: -1014.90 meV to -62.69 meV
     hydro 2 s 2.1
     hydro 2 p 3.5
#  "Second tier" - improvements: -12.89 meV to -1.83 meV
```

```
     hydro 1 s 0.85
     hydro 2 p 3.7
     hydro 2 s 1.2
     hydro 3 d 7
###############################################################
#
#  FHI-aims code project
# Volker Blum, Fritz Haber Institute Berlin, 2009
#
#   Suggested "tight" defaults for C atom (to be pasted into
control.in file)
#
###############################################################
  species        C
#     global species definitions
    nucleus             6
    mass                12.0107
#
    l_hartree           6
#
    cut_pot             4.0  2.0  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         34 7.0
    radial_multiplier   2
    angular_grids specified
      division   0.2187   50
      division   0.4416  110
      division   0.6335  194
      division   0.7727  302
      division   0.8772  434
#      division   0.9334  590
#      division   0.9924  770
#      division   1.0230  974
#      division   1.5020 1202
#     outer_grid  974
      outer_grid  434
##############################################################
#
#  Definition of "minimal" basis
#
###############################################################
#     valence basis states
    valence      2  s   2.
    valence      2  p   2.
#     ion occupancy
    ion_occ      2  s   1.
```

```
    ion_occ      2  p   1.
################################################################
#
#    Suggested  additional  basis  functions.  For  production
calculations,
#   uncomment  them  one  after  another  (the  most  important  basis
functions are
#  listed first).
#
#  Constructed for dimers: 1.0 A, 1.25 A, 1.5 A, 2.0 A, 3.0 A
#
################################################################
#  "First tier" - improvements: -1214.57 meV to -155.61 meV
     hydro 2 p 1.7
     hydro 3 d 6
     hydro 2 s 4.9
#  "Second tier" - improvements: -67.75 meV to -5.23 meV
     hydro 4 f 9.8
     hydro 3 p 5.2
     hydro 3 s 4.3
     hydro 5 g 14.4
     hydro 3 d 6.2
###############################################################
#
#  FHI-aims code project
# Volker Blum, Fritz Haber Institute Berlin, 2009
#
#   Suggested  "tight"  defaults  for  N  atom  (to  be  pasted  into
control.in file)
#
##############################################################
  species        N
#     global species definitions
    nucleus             7
    mass                14.0067
#
    l_hartree           6
#
    cut_pot             4.0  2.0  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         35 7.0
    radial_multiplier   2
    angular_grids       specified
      division   0.1841   50
      division   0.3514  110
      division   0.5126  194
```

```
      division   0.6292  302
      division   0.6939  434
#      division   0.7396  590
#      division   0.7632  770
#      division   0.8122  974
#      division   1.1604 1202
#      outer_grid  974
      outer_grid  434
############################################################
#
#  Definition of "minimal" basis
#
#############################################################
#     valence basis states
    valence      2  s   2.
    valence      2  p   3.
#     ion occupancy
    ion_occ      2  s   1.
    ion_occ      2  p   2.
############################################################
#
#     Suggested additional basis functions. For production
calculations,
#   uncomment them one after another (the most important basis
functions are
#  listed first).
#
#  Constructed for dimers: 1.0 A, 1.1 A, 1.5 A, 2.0 A, 3.0 A
#
############################################################
#  "First tier" - improvements: -1193.42 meV to -220.60 meV
     hydro 2 p 1.8
     hydro 3 d 6.8
     hydro 3 s 5.8
#  "Second tier" - improvements: -80.21 meV to -6.86 meV
     hydro 4 f 10.8
     hydro 3 p 5.8
     hydro 1 s 0.8
     hydro 5 g 16
     hydro 3 d 4.9
#############################################################
#
#  FHI-aims code project
# Volker Blum, Fritz Haber Institute Berlin, 2009
#
#   Suggested "tight" defaults for S atom (to be pasted into
control.in file)
```

```
#
#   Revised Jan 04, 2011, following tests (SiC) done by Lydia
Nemec:
#     d and g functions of tier 2 now enabled by default.
#
###############################################################
  species        S
#     global species definitions
    nucleus             16
    mass                32.065
#
    l_hartree           6
#
    cut_pot             4.0          2.0  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         44 7.0
    radial_multiplier   2
    angular_grids       specified
      division   0.4665  110
      division   0.5810  194
      division   0.7139  302
      division   0.8274  434
#      division   0.9105  590
#      division   1.0975  770
#      division   1.2028  974
#      outer_grid  974
      outer grid  434
###############################################################
#
#  Definition of "minimal" basis
#
###############################################################
#     valence basis states
    valence      3  s   2.
    valence      3  p   4.
#     ion occupancy
    ion_occ      3  s   1.
    ion occ      3  p   3.
###############################################################
#
#     Suggested additional basis functions. For production
calculations,
#   uncomment them one after another (the most important basis
functions are
#  listed first).
#
```

```
#  Constructed for dimers: 1.6 A, 1.9 A, 2.5 A, 3.25 A, 4.0 A
################################################################
#  "First tier" - improvements: -652.81 meV to -45.53 meV
     ionic 3 d auto
     hydro 2 p 1.8
     hydro 4 f 7
     ionic 3 s auto
#  "Second tier" - improvements: -30.20 meV to -1.74 meV
     hydro 4 d 6.2
     hydro 5 g 10.8
#     hydro 4 p 4.9
#     hydro 5 f 10
#     hydro 1 s 0.8
```

Geometries of the most stable polymorphs

PPz herringbone coplanar

86
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.40340153	-0.00056017	7.29648936
Au	0.11089622	0.03496791	9.68702144
Au	2.58823112	1.49133313	9.61960314
Au	0.86506009	1.41383511	7.17989371
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.38343225	2.90963901	7.13663147
Au	-0.00545059	2.95060946	9.44905972
Au	2.54873710	4.38760701	9.47186208
Au	0.83471498	4.45572150	7.15897110
Au	1.69752526	5.88040000	4.80132649

Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.41172159	5.91494779	7.17801922
Au	0.04215144	5.78234718	9.74877361
Au	2.67782545	7.26707275	9.59664743
Au	0.83317232	7.34288895	7.34590691
S	-0.06311018	0.38771379	12.09092276
S	2.31035387	2.31490116	11.90648531
S	4.77382642	5.24949485	12.18096047
S	2.45998514	7.23194758	11.95725039
C	0.47533637	2.77214443	18.23610748
C	1.41790356	3.60895403	18.86797798
C	-0.45709678	2.10450020	19.05753015
C	1.40867326	3.78838776	20.24960387
C	-0.45857922	2.29446825	20.43621781
C	0.47047246	3.13699578	21.04789692
C	-0.23478826	1.31517944	14.82235626
C	-0.04476912	1.35895385	16.32764882
C	1.64977573	3.04875810	16.11743624
C	1.50630931	3.00927454	14.60598041
C	1.05818711	1.49472813	12.73920118
C	3.09093781	6.87198480	18.45500225
C	2.16260076	7.78423567	19.00000262
C	4.04032574	6.31249026	19.33132575
C	2.18122792	8.10948127	20.35342739
C	4.04928188	6.64328390	20.68399092
C	3.12478653	7.54430721	21.21125065
C	4.09050877	5.44256740	15.09874242
C	4.27459949	5.94281792	16.52253954
C	2.51950866	7.52889760	16.19028784
C	2.28917170	7.05231516	14.77516946
C	3.58289016	6.28648790	12.83219660
H	-1.20753102	1.43562849	18.64404693
H	2.17484889	4.13360107	18.29417298
H	2.15569159	4.44709602	20.69104199
H	-1.20552232	1.76791232	21.02901967
H	-0.45487307	0.28346152	14.52338666
H	-1.10333749	1.92014257	14.51967695
H	-1.01739768	1.14734648	16.77931011
H	0.62987455	0.54348360	16.64316952
H	2.51626752	2.43599483	16.43216496
H	1.88151891	4.08561675	16.38751598
H	0.89191619	3.84073403	14.23165695

H	2.49109938	3.15159640	14.14867483
H	0.46453862	3.27929483	22.12805862
H	4.79120004	5.61290365	18.97733482
H	1.39088921	8.24634495	18.39099836
H	1.44165346	8.81834024	20.72541685
H	4.80990358	6.19194063	21.32012824
H	5.07145023	5.20737843	14.68445692
H	3.53107735	4.49697739	15.11022431
H	4.58863916	5.07562034	17.11118841
H	5.09544695	6.68174098	16.55976343
H	3.17036932	8.42008630	16.17674793
H	1.54769910	7.85715811	16.56035865
H	1.42919372	6.36886846	14.72958131
H	2.03198098	7.92082161	14.15962095
H	3.14376841	7.80763341	22.26828624
N	0.94935575	1.76123404	14.09374218
N	0.44678433	2.63325722	16.82792657
N	3.46070427	6.39828670	14.20281710
N	3.05522689	6.51520845	17.08522221

PPz herringbone twisted

86
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.39323008	0.01448273	7.31209888
Au	0.08768031	0.06930593	9.68047143
Au	2.56644025	1.53425783	9.63555550
Au	0.85843332	1.42694351	7.18076815
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.37548457	2.91882899	7.13682682
Au	-0.01952351	2.97299953	9.44502783
Au	2.52834239	4.41937433	9.45652601
Au	0.82825497	4.46381827	7.14629144
Au	1.69752526	5.88040000	4.80132649

Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.40357429	5.93776724	7.18035901
Au	0.01608082	5.82723522	9.70142782
Au	2.64192868	7.31031549	9.62707758
Au	0.83203835	7.35965804	7.33924114
S	-0.08208961	0.37239321	12.08253821
S	2.28050365	2.31841192	11.94198542
S	4.76668268	5.21306873	12.08285451
S	2.44351082	7.20706283	12.00406919
C	0.61680243	2.30345577	18.33089297
C	1.59146540	1.57573801	19.03011924
C	-0.35130238	3.00721894	19.05304398
C	1.60571347	1.57892245	20.42417350
C	-0.33152602	3.02001793	20.44700919
C	0.65093118	2.30816204	21.13666533
C	-0.16165491	1.08780996	14.86308200
C	0.07296788	1.05938921	16.36208602
C	1.81829036	2.65868942	16.23556439
C	1.63296495	2.77702337	14.73322224
C	1.06362010	1.43575979	12.76137177
C	3.21780953	6.29272488	18.44287164
C	2.24253533	5.70720921	19.25593426
C	4.17236501	7.13930512	19.02586319
C	2.21800144	5.95796441	20.62703169
C	4.14442497	7.39543931	20.39613360
C	3.16781605	6.80518173	21.20115924
C	4.21303896	5.25833936	14.96994241
C	4.44253519	5.68601567	16.40528883
C	2.62948336	7.18299001	16.30257260
C	2.37582135	6.90367925	14.83269267
C	3.58820107	6.22575329	12.80102218
H	-1.12416014	3.54571904	18.51050026
H	2.35088206	1.00384657	18.49727559
H	2.37383582	1.01154610	20.94848865
H	-1.08924260	3.59005563	20.98366588
H	-0.35901333	0.06817250	14.50910293
H	-1.05500003	1.68211749	14.62287088
H	-0.86966861	0.81033687	16.86228890
H	0.78692214	0.24965523	16.60469643
H	2.58940993	1.89441785	16.44631388
H	2.18623374	3.62148888	16.61597682
H	1.05613941	3.67741150	14.48643538

H	2.60399833	2.90254949	14.24297515
H	0.67288302	2.31873205	22.22686236
H	4.94882976	7.60386514	18.42021312
H	1.50315196	5.04987249	18.80315896
H	1.44756332	5.48945986	21.23854937
H	4.89311596	8.05934757	20.82775366
H	5.16932702	5.08122414	14.47238213
H	3.67481944	4.29977119	14.95808682
H	4.90709246	4.84890162	16.93646938
H	5.14178920	6.54123698	16.42363457
H	3.31333166	8.04652086	16.39458603
H	1.68527536	7.47806481	16.77014640
H	1.47959533	6.28177516	14.70707754
H	2.17375856	7.85358750	14.32281350
H	3.14774258	7.00572758	22.27283712
N	0.99223709	1.60966696	14.13276009
N	0.54921272	2.33480951	16.89047072
N	3.51421487	6.25919121	14.17915876
N	3.16470474	6.03032100	17.02701821

PPz cofacial coplanar

86
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.38826236	-0.06565220	7.16269961
Au	0.00167480	0.01027637	9.50297681
Au	2.55680469	1.42581388	9.43110759
Au	0.83592361	1.47406348	7.12552626
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.40433268	2.97695057	7.18901899
Au	0.00889171	2.94458574	9.56329340
Au	2.54402217	4.34227986	9.72975591
Au	0.84599046	4.41139181	7.26229252
Au	1.69752526	5.88040000	4.80132649

Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.36326913	5.85217220	7.34102730
Au	0.03584594	5.93865237	9.61190623
Au	2.54832923	7.39586721	9.68414014
Au	0.85326273	7.31070701	7.19263873
S	0.16073277	1.95195727	11.77988827
S	2.62458539	3.72152380	12.14398685
S	-0.03687743	5.91564181	11.99863234
S	2.39950360	7.74025235	12.11309347
C	1.56321948	1.20495778	18.17750891
C	2.49466314	1.77307879	19.06928837
C	0.55976035	0.38332715	18.73212385
C	2.43845283	1.50534396	20.43257669
C	0.51610081	0.11885325	20.09705608
C	1.45474777	0.67254171	20.96406059
C	0.83137235	1.00556728	14.49475618
C	0.48615566	1.19763019	15.96086528
C	2.42280952	2.53570454	16.28576801
C	2.76448828	2.37428858	14.80883294
C	1.48859234	2.56984765	12.67995874
C	1.54677714	5.58574024	18.38141402
C	2.51962090	6.17985627	19.20949063
C	0.59043605	4.75681167	19.00245066
C	2.53933404	5.93907224	20.57847855
C	0.62189748	4.51961451	20.37271238
C	1.59532519	5.10546512	21.17820620
C	0.62438563	5.30389830	14.75103333
C	0.35208159	5.47106037	16.23356838
C	2.21470175	6.93592701	16.41805460
C	2.52358077	6.74112496	14.94145381
C	1.24897837	6.68458109	12.80936471
H	-0.21175229	-0.05854913	18.10741896
H	3.27759750	2.43704557	18.71571800
H	3.18085841	1.96469254	21.08406902
H	-0.27151343	-0.52864504	20.47922453
H	1.42962275	0.09562885	14.36485029
H	-0.07015444	0.86924620	13.89164373
H	-0.17572982	2.07065583	16.06756004
H	-0.07703941	0.31720365	16.28516549
H	3.36262899	2.61897051	16.83605677
H	1.88807713	3.48304795	16.45584470
H	3.29723701	3.25566848	14.43802764

H	3.42445190	1.50608028	14.68268422
H	1.41841428	0.46121104	22.03169441
H	-0.20427331	4.28964323	18.42866733
H	3.27444046	6.84419202	18.79937987
H	3.31228197	6.41508925	21.18086048
H	-0.13443503	3.86647310	20.80595661
H	1.23812370	4.40850701	14.58559599
H	-0.30883071	5.13548797	14.20860542
H	-0.38911239	6.27025925	16.39664293
H	-0.10139447	4.53744385	16.58140064
H	3.15394480	7.13242257	16.93961777
H	1.59715658	7.83390623	16.55849457
H	3.02691204	7.62221507	14.53170792
H	3.20706040	5.88949435	14.81941230
H	1.61755621	4.91877180	22.25096321
N	1.58426629	2.14213316	13.98445725
N	1.67074954	1.39159344	16.78461459
N	1.31222810	6.45758697	14.17438052
N	1.56617974	5.75823474	16.98300709

PPz cofacial twisted

86
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.37828339	-0.05407188	7.15682849
Au	-0.01600399	0.01906964	9.48741336
Au	2.54371625	1.44138943	9.43850297
Au	0.83236654	1.48437000	7.12783377
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.40394258	2.98392094	7.19532099
Au	-0.00312077	2.94058068	9.58667320
Au	2.52888291	4.35726637	9.72400632
Au	0.84033281	4.41571687	7.27595134
Au	1.69752526	5.88040000	4.80132649

Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.36163530	5.85943991	7.34009606
Au	0.01579408	5.94635163	9.62898766
Au	2.52936350	7.40828718	9.67055025
Au	0.84732530	7.31032601	7.18981203
S	0.16353702	2.02031352	11.83662338
S	2.61792370	3.81174233	12.13470198
S	-0.04756349	5.98834428	12.02446247
S	2.37561186	7.83353624	12.08250303
C	1.57810136	1.66734156	18.24510657
C	0.54996640	2.39834118	18.85532280
C	2.49943562	0.99666248	19.05740738
C	0.44454967	2.45377173	20.24304641
C	2.39464719	1.05110087	20.44475924
C	1.36527866	1.77883512	21.04359273
C	0.85782381	1.15787202	14.58293896
C	0.52592190	1.43461104	16.04310111
C	2.47934019	2.74770051	16.28522955
C	2.80928563	2.53873904	14.81453563
C	1.49119480	2.66690556	12.70785840
C	1.48999521	6.07086637	18.41298854
C	0.48333436	6.81961238	19.03753480
C	2.43077104	5.40734082	19.20709647
C	0.41990990	6.89912733	20.42648287
C	2.36782207	5.48704948	20.59633055
C	1.36108079	6.23251131	21.21122194
C	0.62978416	5.45611318	14.80032290
C	0.36213347	5.72239640	16.27209639
C	2.25243567	7.14194318	16.38438194
C	2.55039337	6.89405892	14.91504479
C	1.24074436	6.78028206	12.80867806
H	3.29779734	0.42909796	18.58369476
H	-0.16956656	2.94269763	18.24707562
H	-0.35960679	3.03237733	20.69546098
H	3.11780326	0.51593745	21.05880106
H	1.45180035	0.24049163	14.49788354
H	-0.04336875	1.00064546	13.98496357
H	-0.09224985	2.34523316	16.08503936
H	-0.06871666	0.60527078	16.45136236
H	3.40893644	2.86381813	16.85087481
H	1.92256412	3.68809123	16.42938942
H	3.32947236	3.40833106	14.40043541

H	3.47152481	1.67000639	14.71377863
H	1.28059226	1.81984060	22.12957637
H	3.20696219	4.82143651	18.71905814
H	-0.25491566	7.35171307	18.43983437
H	-0.36848420	7.48758542	20.89355828
H	3.10605458	4.95923458	21.19894447
H	1.23373270	4.54728761	14.68180350
H	-0.30185883	5.27490943	14.25971819
H	-0.32366508	6.58145871	16.35401658
H	-0.14523954	4.85285073	16.71165629
H	3.18553482	7.34999662	16.91882275
H	1.63155751	8.04436809	16.49898131
H	3.04729291	7.75658049	14.45993501
H	3.23127087	6.03802877	14.82221514
H	1.30881238	6.29347993	22.29844114
N	1.61421639	2.27011901	14.02045160
N	1.75052501	1.59425187	16.82236365
N	1.32939266	6.57791301	14.17425795
N	1.61292616	5.96752950	16.98554960

PPd herringbone coplanar

88
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.36745273	-0.02681347	7.14237564
Au	-0.03293871	0.03048354	9.45744036
Au	2.51631425	1.46821549	9.45093568
Au	0.82422343	1.50050797	7.12953290
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.40287716	2.99728468	7.21250164
Au	-0.04953324	2.92787702	9.62486869
Au	2.46442515	4.37795657	9.70815610
Au	0.83435059	4.42158302	7.28945586
Au	1.69752526	5.88040000	4.80132649

Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.35882906	5.87673235	7.29326516
Au	-0.09056267	5.95621833	9.61585252
Au	2.49717718	7.42641489	9.68183592
Au	0.85702959	7.31501371	7.21159187
S	0.24657870	2.10852389	11.91013452
S	2.59764284	4.05364735	12.13206764
S	5.15652852	6.06022154	11.99179300
S	2.82727479	8.04480278	12.06617621
C	1.60490122	2.00773510	18.50306969
C	2.48788955	2.69035893	19.35382031
C	0.58974209	1.24546949	19.10162741
C	2.37397999	2.59408176	20.74000871
C	0.47508373	1.13867090	20.48713891
C	1.37248116	1.81100270	21.31514840
C	0.76244374	1.64743760	14.70540105
C	0.52199201	1.73296558	16.20121921
C	2.32510847	3.34812138	16.44729420
C	2.55820358	3.35863383	14.93648233
C	1.43093777	2.99554239	12.77955364
C	4.07180780	6.62272975	18.57900099
C	3.07127559	7.23068300	19.35189292
C	4.93119277	5.71835072	19.22253212
C	2.93502124	6.95244278	20.71139606
C	4.80092594	5.43715222	20.58198462
C	3.80131764	6.05440295	21.33437148
C	5.12637719	6.23369023	14.81509855
C	4.87960201	5.88162590	16.27440390
C	2.99325109	7.40455811	16.38374086
C	3.27618608	7.88399801	14.96849770
C	3.97752967	7.00361199	12.78789378
H	-0.13942470	0.71921196	18.49074238
H	3.29208854	3.30053223	18.94645435
H	3.08376206	3.13165830	21.36688552
H	-0.32442459	0.52941582	20.90733922
H	1.33179138	0.73735458	14.45915876
H	-0.18659233	1.54407289	14.16568118
H	-0.21169639	2.51985823	16.42370951
H	0.06778033	0.78451080	16.50430383
H	3.27144807	3.60800606	16.93191102
H	1.61727239	4.13461069	16.72574514
H	2.72711749	4.38630930	14.59074522

H	3.47972606	2.80798618	14.68861694
H	1.28956068	1.73023362	22.39940106
H	5.73463256	5.22721319	18.67653429
H	2.37913930	7.94149320	18.90475783
H	2.13963843	7.44016899	21.27397171
H	5.49050914	4.73082020	21.04340708
H	6.02964400	6.85244121	14.71282701
H	5.32757003	5.31363939	14.25431342
H	4.23029372	5.00320900	16.33311846
H	5.84133778	5.58212640	16.69299224
H	2.44752194	8.19564619	16.90795966
H	2.32739661	6.53405376	16.35132392
H	2.34425586	8.08657789	14.43156365
H	3.81636404	8.84616960	14.99732829
H	3.69472808	5.83332325	22.39686824
N	1.44567551	2.81379420	14.15262114
N	4.00659282	6.91630843	14.16583659
C	1.79133182	2.02912374	16.99069445
H	2.53773872	1.25247016	16.74868550
C	4.26658687	6.99261710	17.11476671
H	4.96967963	7.84555655	17.09659755

PPd herringbone twisted

88

Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.36418120	-0.02666824	7.12572316
Au	-0.03814642	0.00871494	9.44128616
Au	2.49471907	1.44908341	9.45388205
Au	0.81443495	1.50066748	7.13857253
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.39343728	2.98039748	7.21396203
Au	-0.07185799	2.87637030	9.67599172
Au	2.43852001	4.34282140	9.64338460

Au	0.80428919	4.41507857	7.29985365
Au	1.69752526	5.88040000	4.80132649
Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.36840413	5.86612807	7.29411538
Au	-0.09181828	5.92321411	9.70100197
Au	2.48861055	7.36855378	9.61545914
Au	0.84840997	7.29515775	7.20635579
S	0.18777043	2.21424864	12.04814945
S	2.53004782	4.18663413	12.03418497
S	2.80493903	8.23026350	11.88277260
S	5.12062719	6.23699898	12.12098092
C	1.46752613	3.48713306	18.57748060
C	0.45511680	4.34811607	19.02726722
C	2.34105197	2.94363118	19.52717902
C	0.33420553	4.67360182	20.37736395
C	2.22282789	3.25989715	20.88024070
C	1.22144024	4.13204556	21.30946056
C	0.62787824	2.27511498	14.96526324
C	0.38274112	2.71996079	16.40221803
C	2.22128001	4.31170046	16.30388744
C	2.45717366	3.97524970	14.83873720
C	1.33791051	3.22799477	12.80233288
C	3.74704984	7.91774953	18.48668194
C	4.72269668	8.77409692	19.01865370
C	2.81053826	7.35903933	19.36571615
C	4.74463505	9.08413334	20.37773790
C	2.83066460	7.65849024	20.72752387
C	3.79452260	8.52951113	21.23721637
C	2.99392389	8.41766177	14.68921930
C	3.15728572	8.75448232	16.16572236
C	4.99301290	7.18158029	16.38683165
C	4.82607187	6.69405468	14.95633040
C	4.02328482	7.38081403	12.74447302
H	3.12657922	2.26074671	19.20364260
H	-0.26601500	4.76946197	18.32740445
H	-0.45933003	5.34917619	20.69441796
H	2.92442409	2.82491663	21.59185714
H	1.16819338	1.31524962	14.94981082
H	-0.31555497	2.07971386	14.44128750
H	-0.32098542	3.56177345	16.40577875
H	-0.09955227	1.91067488	16.95881615
H	3.16732355	4.66059801	16.73490359

H	1.52235230	5.15170796	16.37543074
H	2.62175911	4.89831545	14.27007992
H	3.38107209	3.38851708	14.72042073
H	1.12768551	4.38702191	22.36552053
H	2.05202945	6.67743775	18.98088063
H	5.49337670	9.20197842	18.37847294
H	5.50950478	9.76029862	20.75804928
H	2.08284745	7.21148366	21.38181156
H	2.03941029	7.89471861	14.52018389
H	2.92352810	9.34436415	14.10393260
H	3.85206549	9.59146488	16.27649804
H	2.19160583	9.10720973	16.54357590
H	5.46445667	6.39140644	16.98045578
H	5.67717413	8.03920574	16.41088193
H	5.80038148	6.52668842	14.48223723
H	4.33686314	5.70629256	14.94922963
H	3.80981457	8.77159500	22.30025971
N	1.35153504	3.27536465	14.18433076
N	4.08067517	7.62525012	14.10434122
C	1.66099937	3.14822768	17.11615943
H	2.38314975	2.32024243	17.07505586
C	3.66535416	7.59157585	17.01220508
H	2.95784192	6.75713734	16.90881506

PPd cofacial coplanar

88
Lattice="5.09257578 0.0 0.0 0.0 8.8206 0.0 0.0 0.0 47.0"
Properties=species:S:1:pos:R:3 pbc="T T T"

Au	1.69752526	0.00000000	4.80132649
Au	4.24381315	1.47010000	4.80132649
Au	3.39505052	0.00000000	0.00000000
Au	0.00000000	0.00000000	2.40066325
Au	2.54628789	1.47010000	2.40066325
Au	0.84876263	1.47010000	0.00000000
Au	3.38006983	-0.04757363	7.15494169
Au	-0.01515721	0.03029132	9.48732715
Au	2.54906340	1.45143967	9.43668624
Au	0.83432227	1.49065667	7.12786829
Au	1.69752526	2.94020000	4.80132649
Au	4.24381315	4.41030000	4.80132649
Au	3.39505052	2.94020000	0.00000000
Au	0.00000000	2.94020000	2.40066325
Au	2.54628789	4.41030000	2.40066325
Au	0.84876263	4.41030000	0.00000000
Au	3.40752463	2.98959312	7.19252508

Au	-0.00019534	2.95038807	9.58621047
Au	2.53030344	4.37300129	9.70409793
Au	0.84231282	4.42407745	7.27492577
Au	1.69752526	5.88040000	4.80132649
Au	4.24381315	7.35050000	4.80132649
Au	3.39505052	5.88040000	0.00000000
Au	0.00000000	5.88040000	2.40066325
Au	2.54628789	7.35050000	2.40066325
Au	0.84876263	7.35050000	0.00000000
Au	3.36855632	5.86834551	7.33592570
Au	0.01243313	5.96008289	9.64132821
Au	2.52737373	7.41861566	9.66504258
Au	0.84800292	7.31548824	7.19194928
S	0.19681847	2.04106174	11.84018228
S	2.64146673	3.85114654	12.10314632
S	-0.03529033	5.99285786	12.04513169
S	2.38223860	7.84105483	12.07358177
C	1.40988144	2.11993740	18.34156748
C	2.15789477	3.01268219	19.12214944
C	0.30621103	1.50135847	18.94801710
C	1.82453510	3.27430341	20.44934210
C	-0.03055818	1.75666504	20.27565853
C	0.72620597	2.64708682	21.03477199
C	0.97687194	1.15147969	14.56485674
C	0.62202454	1.42765679	16.02204709
C	2.59995246	2.88286123	16.20734438
C	2.92224111	2.53580589	14.75661055
C	1.54553766	2.68022278	12.68530411
C	1.29322668	6.52223046	18.56042668
C	2.09490460	7.41075639	19.29240622
C	0.19985721	5.94480214	19.22120020
C	1.82209122	7.70519164	20.62588008
C	-0.07573939	6.23292193	20.55663012
C	0.73317129	7.11708793	21.26740788
C	0.68347421	5.45376790	14.82024403
C	0.43084143	5.67327171	16.31182305
C	2.31176749	7.27154765	16.34314801
C	2.60533385	6.88675217	14.90054842
C	1.26140317	6.78091475	12.81713159
H	-0.29662618	0.78680099	18.39070064
H	3.02982852	3.50802905	18.70107621
H	2.42140022	3.98470748	21.02044640
H	-0.89268648	1.25600190	20.71280690
H	1.59432485	0.24947324	14.47255388
H	0.08333538	0.96365016	13.96315706
H	-0.06158965	2.28048736	16.05749518

H	0.06329547	0.56229617	16.40506549
H	3.53405615	3.10284007	16.73748983
H	2.00950961	3.79830775	16.22830011
H	3.48701135	3.33456526	14.26627359
H	3.53828121	1.62632925	14.71618895
H	0.45693671	2.85811571	22.06975533
H	-0.44332285	5.23816491	18.70046831
H	2.95951612	7.87954593	18.82776996
H	2.45941651	8.40952125	21.15943616
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H	1.27774952	4.54664198	14.64615946
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H	3.24637845	7.59213335	16.82102487
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C	1.64416191	6.14603340	17.12723314
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PPd cofacial twisted

88
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Au	0.84876263	1.47010000	0.00000000
Au	3.37584310	-0.04245676	7.14901482
Au	-0.02388554	0.02961458	9.47766713
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Au	3.36807786	5.86866588	7.33414083
Au	-0.00223571	5.95744729	9.65570914
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Au	0.84352360	7.31226584	7.18890724
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C	1.74576856	1.98754729	18.39518701
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H	2.67097003	0.91955388	16.83390467
C	1.82471481	6.15919770	17.08096173
H	2.54767817	5.33661372	17.02861342

References

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