Supplementary Information

Controlling Pairing of π-Conjugated Electrons in 2D Covalent Organic Radical Frameworks via In-plane Strain

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Section 1. Results at 0K

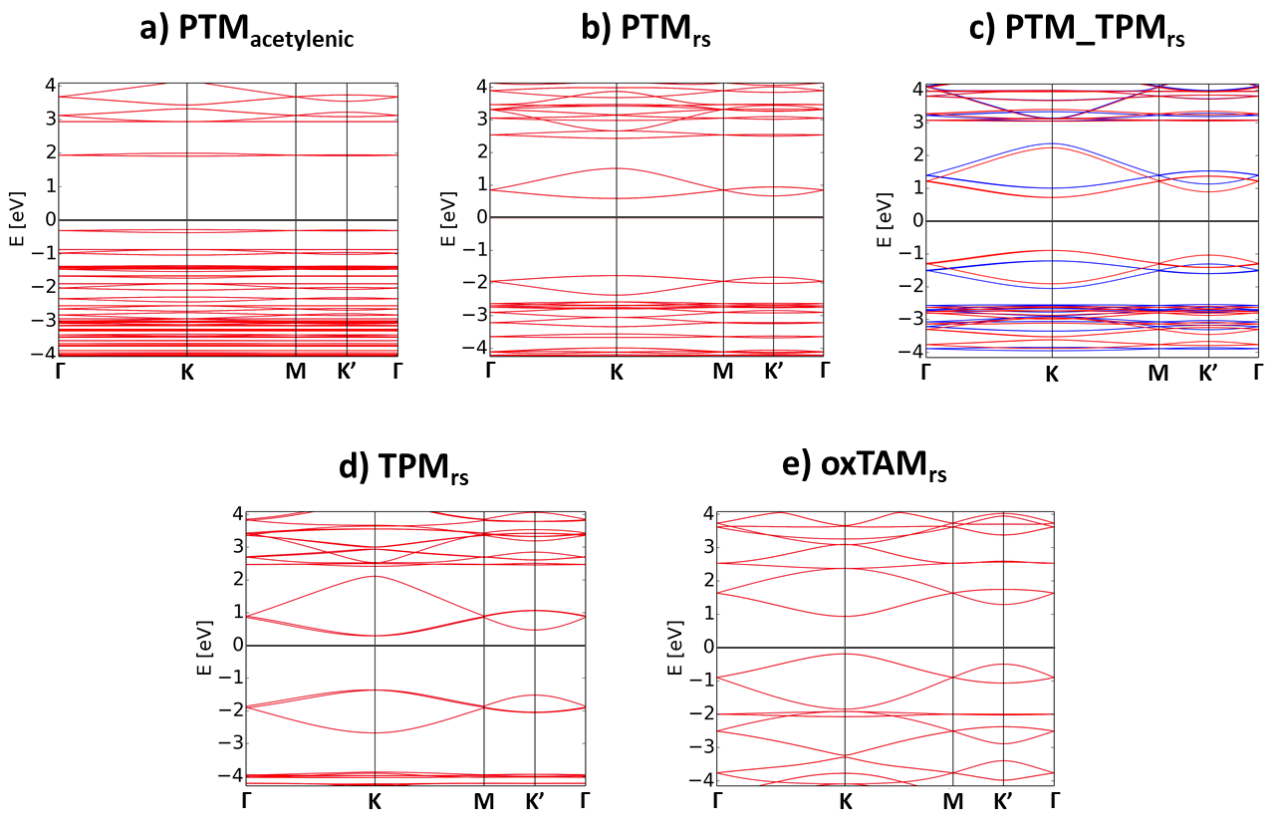


Fig. S1. Spin-resolved (spin-up: blue; spin-down: red) band structures for the (AFM) open-shell electronic solution of the 2D-CORFs considered in this work. Note that in band structures **a)**, **b)**, **d)** and **e)** spin-up and spin-down bands are exactly superimposed. For **c)**, due to the different chemical functionalization of *A* (chlorinated aryl rings) and *B* (hydrogenated aryl rings) lattices, the AFM spin degeneracy is lifted. The Fermi level is indicated with a horizontal black line.

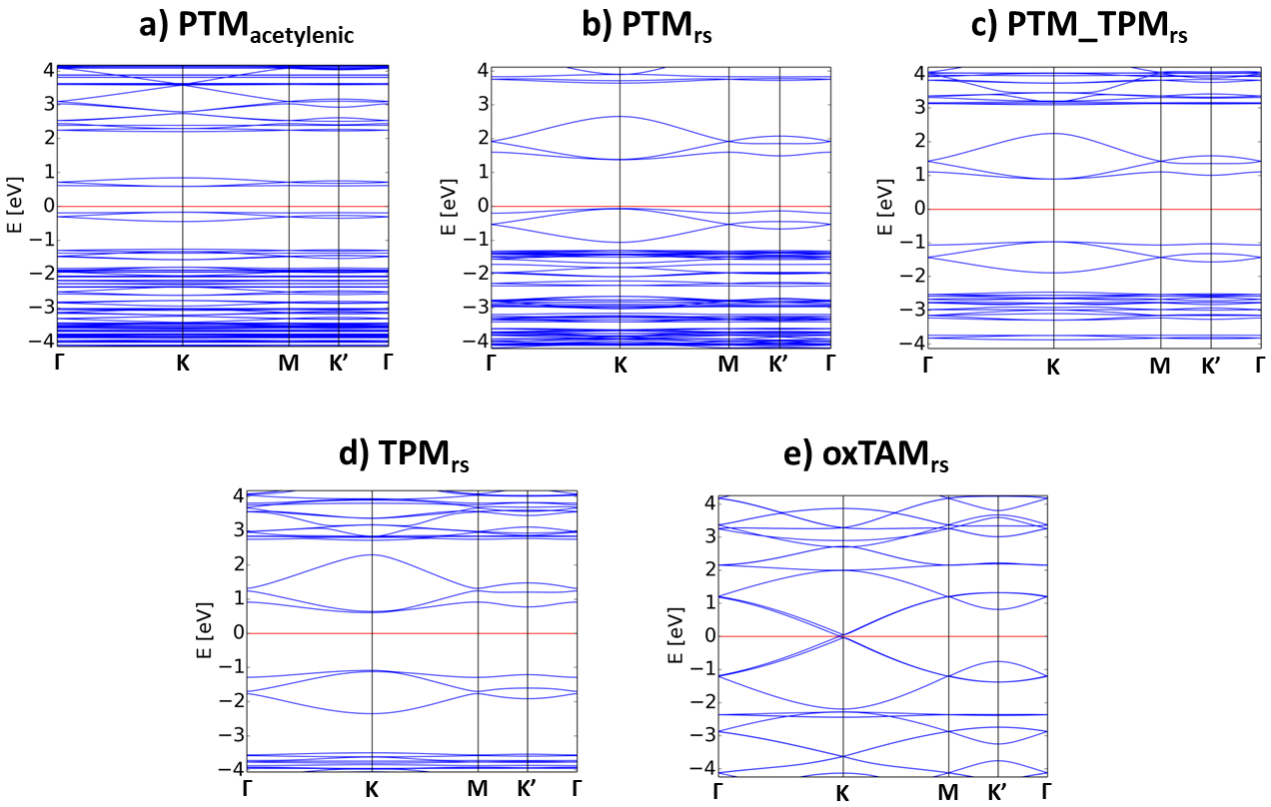


Fig. S2. Band structures for the closed-shell (quinoidal) electronic solution of the 2D-CORFs considered in this work. The presence of a semimetallic Dirac cone for oxTAM$_{rs}$ (**e**) reveals its tendency to favour delocalization as opposed to local electron pairing. The Fermi level is indicated with a horizontal red line.

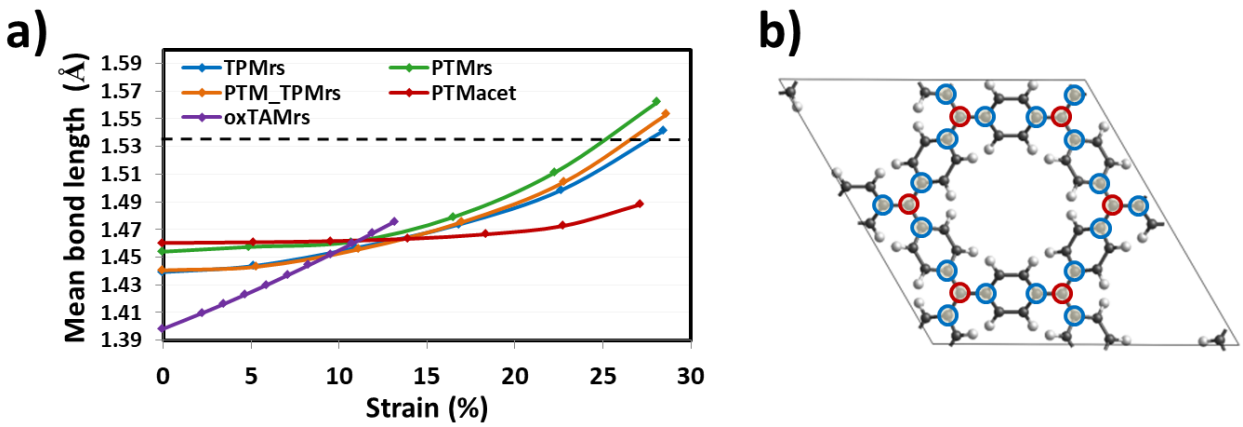


Fig. S3. **a)** Mean bond length (Å) between αC atoms (red circle in **b**) and their first nearest neighbours (blue circle in **b**) against uniaxial strain for all considered 2D-CORFs. The dotted horizontal line is the C-C distance in ethane (1.535Å),[1] as a prototypical length for the single C-C bond.

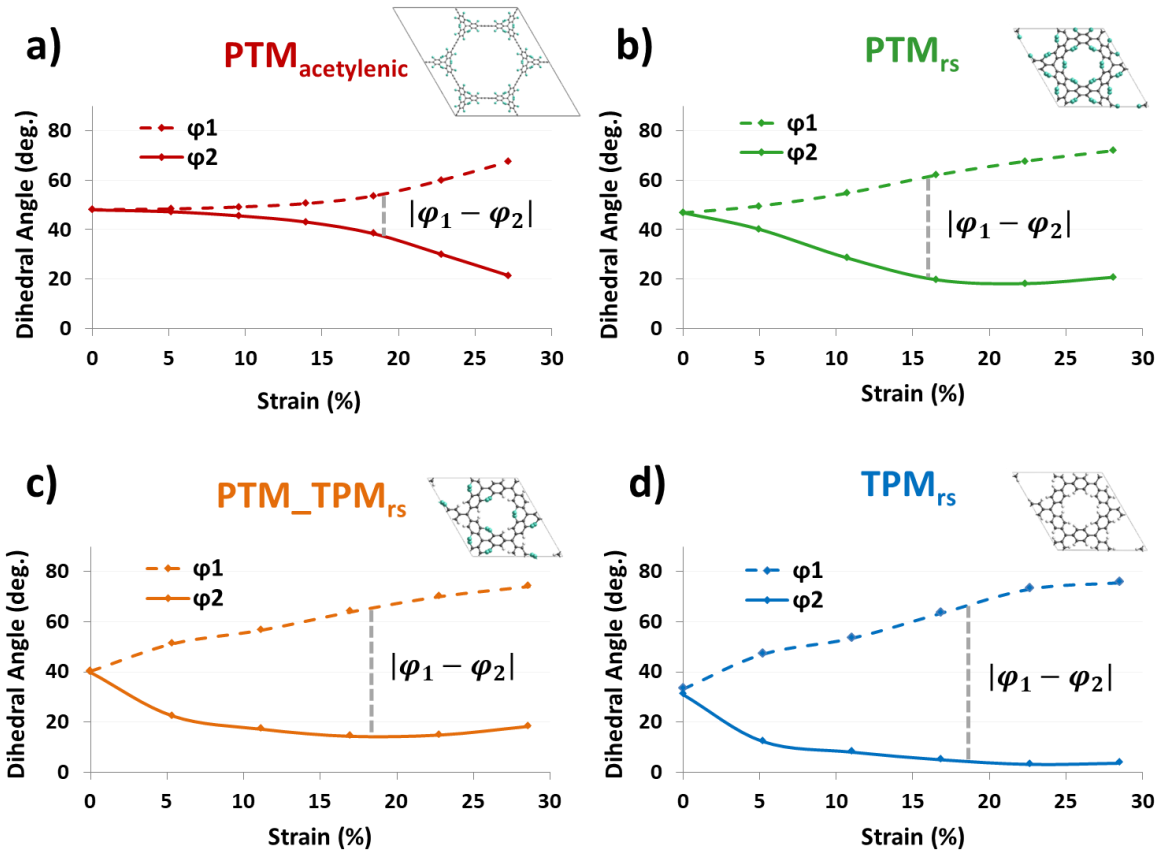
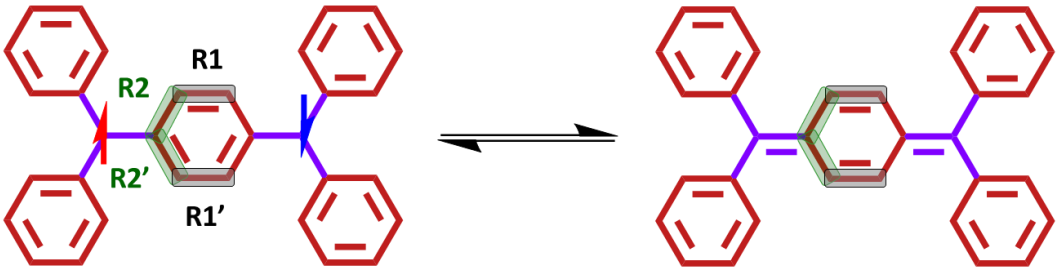


Fig. S4. Dihedral angle (degrees) *vs*. uniaxial strain (%) for the aryl rings parallel (φ_2) and non-parallel (φ_1) to the strain direction. The difference between the two angles ($|\varphi_1 - \varphi_2|$; vertical dashed grey lines) *vs*. strain is presented in **Fig. 3** in the main text.



$$\langle R_1 \rangle = \frac{R_1 + R'_1}{2}$$

$$\langle R_2 \rangle = \frac{R_2 + R'_2}{2}$$

$$BLA = \langle R_2 \rangle - \langle R_1 \rangle$$

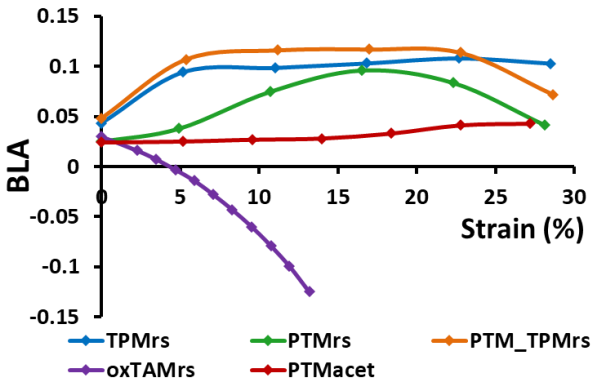


Fig. S5. Bond length alternation (BLA) vs. uniaxial strain calculated from the difference between bond lengths of type R_1 and R_2 within aryl rings accommodating electron pairing (i.e. those parallel to the strain direction).

2D Material	Calculated in-plane Young's Modulus (GPa)	% relative to graphene	Approx. multiplicative factor relative to graphene
$PTM_{acetylenic}$	2.1	0.2	$\frac{1}{458}$
TPM_{rs}	31.4	3.3	$\frac{1}{31}$
PTM_TPM_{rs}	33.4	3.5	$\frac{1}{29}$
PTM_{rs}	46.7	4.9	$\frac{1}{21}$
MoS_2	*265±13(exp)*[2]	27.5±1	$\frac{1}{3.6}$
$oxTAM_{rs}$	651.8	67.7	$\frac{1}{1.5}$
graphene	962.6, *1024(theory)*[3], *1020±150(exp.)*[4]	100	1

Table S1. Comparison of our calculated in-plane Young's Modulus (YM) values for our considered 2D-CORF materials as compared to that of graphene and single layer MoS_2. Our calculated YM values are underlined and YM values from other recent experimental and theoretical studies values (for MoS_2 and graphene) are in italics. For our 2D-CORFs we use a strain range of 0-25% and the supercells reported in the main text. The thickness of each 2D-CORF material is taken to be the sum of the maximal interatomic distance in the out-of-plane direction and twice the van der Waals radius of the outermost atoms. For graphene we use a smaller 0 - 8% range of strain, with an 18 atom (3×3×1) supercell, and take the thickness to be the interlayer separation distance in graphite. In our calculations we use our computed total energy versus strain data which can be well approximated as being in the elastic and linear regime (i.e. Hooke's Law response to strain). Under this approximation we used the relation: $E(\Delta L) = \frac{k}{2}\Delta L^2$ – where ΔL is the elongation with respect to strain (in the stretching direction), $E(\Delta L)$ is the resultant change in total energy with respect to the strain-induced elongation, and k is the spring constant. A quadratic fit to our calculated $E(\Delta L)$ versus ΔL data gives us a value of k, from which we derive the YM values via: $\mathrm{YM} = \frac{kL_0}{A}$, where L_0 is the initial relaxed length of the material and A is the cross sectional area.

2D-CORF	$E_{AFM} - E_{FM}$ (meV/αC)	Magnetic coupling, *J* (meV)
$PTM_{acetylenic}$	-25	-17 *(-15)*
PTM_{rs}	-213	-142 *(-157)*
PTM_TPM_{rs}	-353	-235
TPM_{rs}	-476	-317 *(-318)*
$oxTAM_{rs}$	-555	-370

Table S2. Calculated magnetic couplings (*J*) for all considered 2D-CORFs. The Heisenberg Hamiltonian is given by: $\widehat{H} = -2J\sum_{i>j}\hat{S}_i \cdot \hat{S}_j$ where the sum runs over all different pairs of spins of directly connected centres. If the strong localization limit of the mapping is taken, it is assumed that the diagonal form of the Heisenberg is valid (i.e. the Ising model in which only the $\hat{S}_i^z$ components of the spin operators appear), and thus: $\widehat{H} = -2J\sum_{i>j}\hat{S}_i^z\hat{S}_j^z$. From this 2D model it follows that: $E_{AF} - E_{FM} = 2zS^2J$, where *z* is the number

of nearest neighbours of a given centre connected by *J* and the energies are given per magnetic centre. In the case of our 2D-CORFs, we take an array of S = ½ magnetic centres (i.e. radical αC centres) on the 2D honeycomb lattice where z = 3, we then have: $J = \frac{E_{AF}-E_{FM}}{2zS^2} = \frac{2}{3}(E_{AF} - E_{FM})$. In the table we include calculated $E_{AF} - E_{FM}$ values and the corresponding values of *J* for all considered relaxed (i.e. unstrained) 2D-CORFs. In parentheses we also include values obtained for three 2D-CORFs reported in ref. 8. We note that the present *J* values are based on supercells using six αC centres, rather than supercells using two αC centres in ref. 8. As larger supercells provide more degrees of freedom for structural relaxation, the present J values should be taken as being slightly more refined results.

Section 2. Results at 300K

Fig. S6 presents the dihedral angle variations associated with each aryl ring within the unit cell (nine in total) throughout the 3ps AIMDS runs for TPM_{rs}, PTM_TPM_{rs} and PTM_{rs} at different strains (ε = 0%, 16% and 28%). Overall, all 2D-CORFs present the same global behavior. In the relaxed conformation (ε = 0%) we see that TPM_{rs} (**S6a**) exhibits significantly higher dihedral angle fluctuations than the other two 2D-CORFs. This difference is due to the smaller steric hindrance of phenyl rings (H-functionalized) compared to perchlorinated rings (Cl-functionalized), leading to a higher conformational flexibility within TPM_{rs}. Such differences were also found for the associated triarylmethyl molecules[5] (the triphenylmethyl[6] and perchlorotriarylmethyl,[7] respectively), which points to the generality of this effect. Upon stretching we observe the same behavior as found at 0K (**Fig. 3** in the main text): i.e. aryl rings bridging αC centers along the stretching direction become more planar with strain (see 2 in the structures at the top of **Fig. S6a**) whereas the non-parallel ones get twisted towards higher out-of-plane dihedral angles (see 1 in the structures at the top of **Fig. S6a**). Indeed, for both ε = 17% and 28 % we see there is a dihedral angle splitting for the three 2D-CORFs. For TPM_{rs}, the flattened aryl rings (2) are stabilized into a nearly flat conformation (i.e. dihedral angles fluctuate very close to 0°), whereas the other set of aryl rings become highly perpendicular, with dihedral angles close to 80° (**Fig. S6c**).

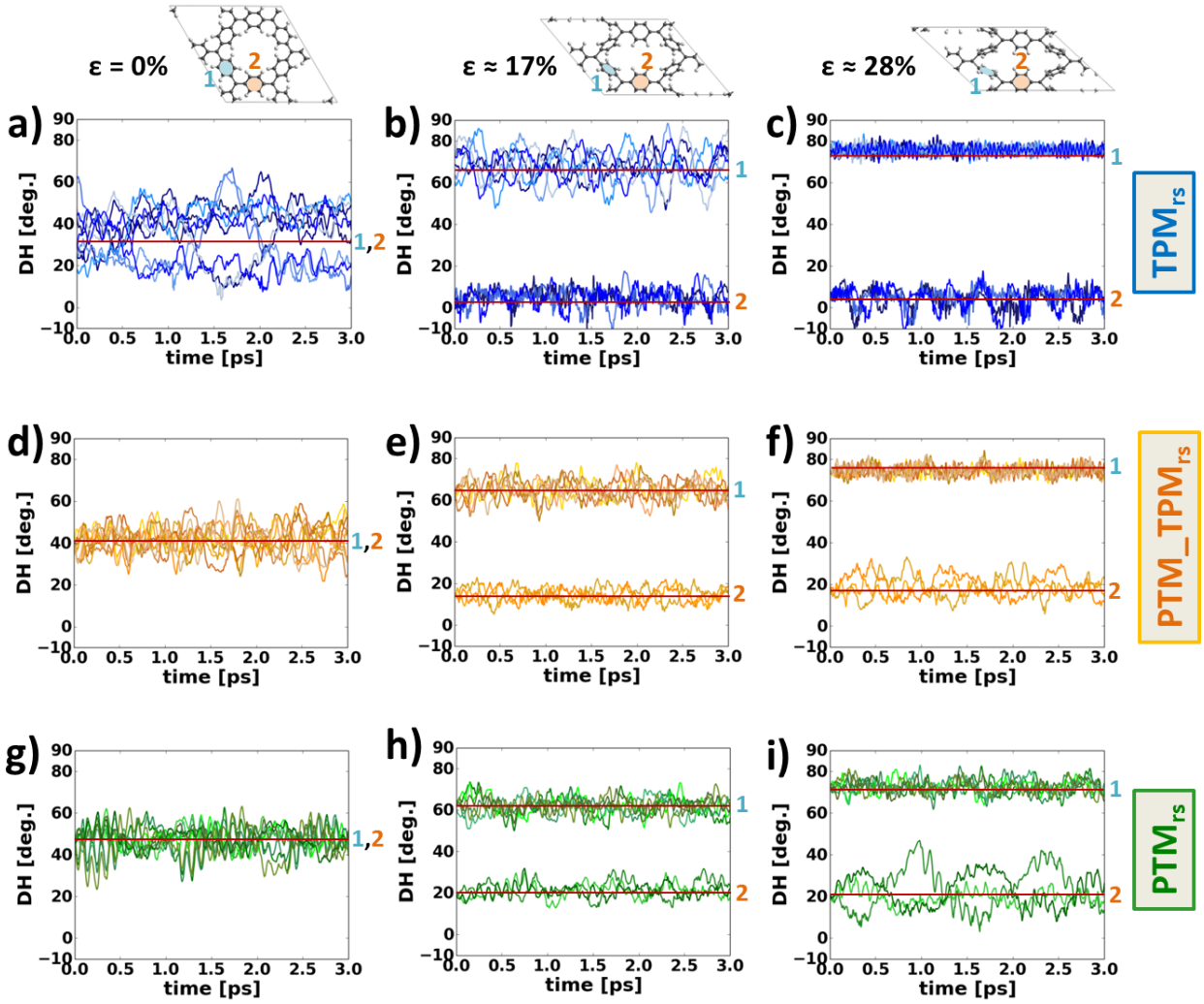


Fig. S6. Time-resolved evolution of dihedral angles (DH) of each of the nine aryl rings within the unit cell during 3ps AIMDS at 300K, at different uniaxial strains (columns) for the **(a, b, c)** TPM_{rs}, **(d, e, f)** PTM_TPM_{rs} and **(g, h, i)** PTM_{rs}. Horizontal red lines indicate the averaged values of aryl ring types 1 and 2 (see inset structures at the top) for the corresponding optimized structures at 0K.

Such general behavior is also found for the PTM_TPM_{rs} and PTM_{rs}, but with lower torsional differences due to the lower conformational flexibility caused by steric hindrance effects, as explained above. Finally, another general trend we observe is the larger rotations for flattened aryl rings for the highest applied strains (ε = 28%) compared with the remaining aryl rings (see **Fig. S6c, f, i**). Once more, the explanation for this effect is steric hindrance. In these highly stretched conformations the two out-of-plane aryl rings are very close to each other, increasing steric hindrance and significantly decreasing their fluctuation freedom. Conversely, flattened aryl rings become further away from the other "out-of-plane" rings with increasing strain, which gives them a higher rotational flexibility (lower steric hindrance). In such "sterically-free" situation, we may see that aryl rings in PTM_{rs} show more significant fluctuations than for the TPM_{rs}, which cannot be explained by steric-hindrance effects. We believe this apparent contradiction shows the effect of the significant weight differences between H atoms and Cl atoms. Cl atoms have a much higher inertia (higher atomic mass) and so their thermal vibrations lead to higher rotational motion, as compared with the lighter (and so less perturbative) H atoms. Overall, results of **Fig. S6** demonstrate that the external manipulation of aryl ring dihedral angles via uniaxial strain operates efficiently under the effect of thermal fluctuations at room temperature (300K).

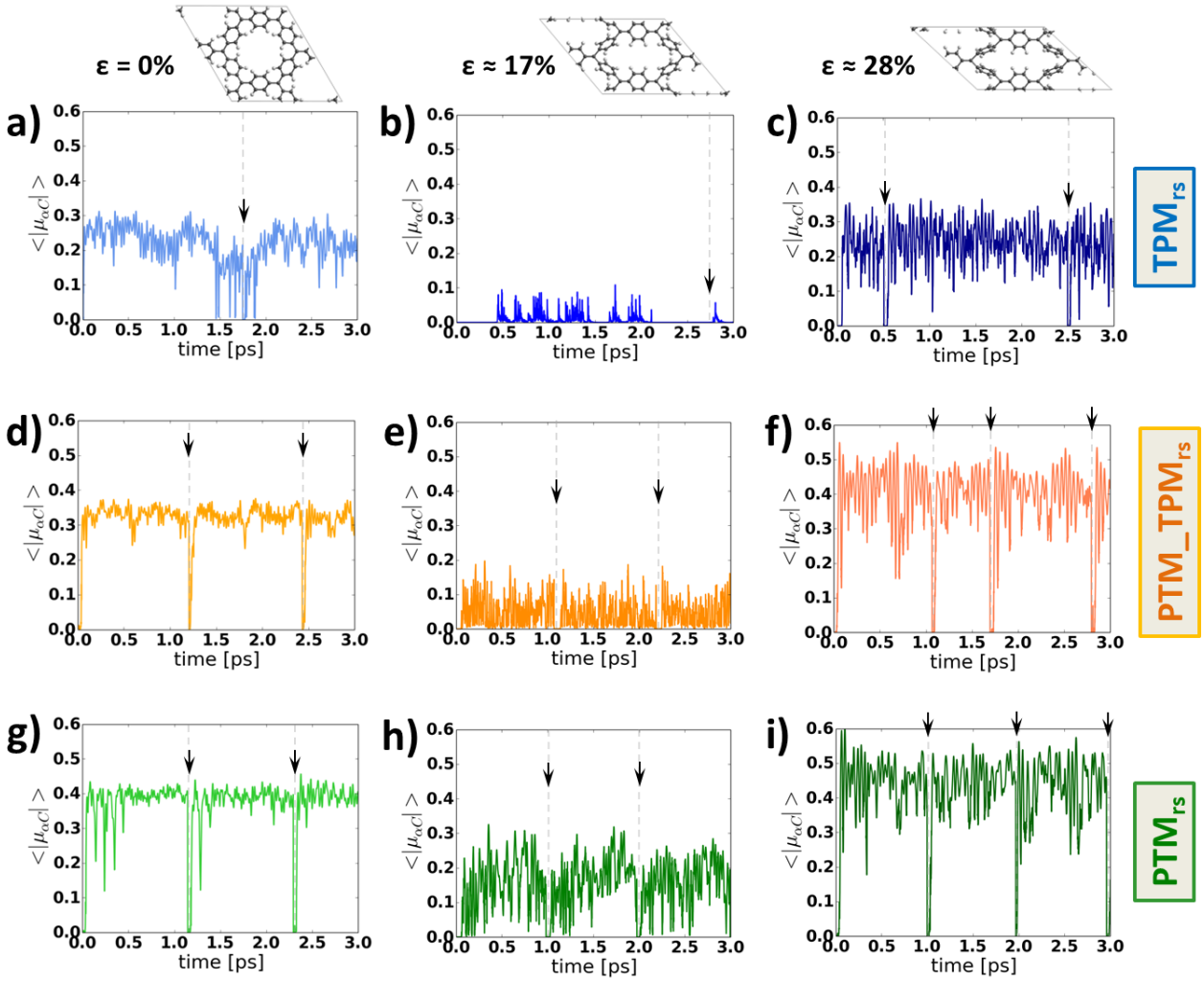


Fig. S7. Time-resolved evolution of αC averaged absolute spin population during 3ps AIMDS at 300K at different uniaxial strains for the **(a, b, c)** TPM_{rs}, **(d, e, f)** PTM_TPM_{rs} and **(g, h, i)** PTM_{rs}. The arrows and dashed lines indicate re-starting points during each AIMDS, causing a sudden (and unphysical) decrease of absolute spin due to the non-spin polarized initial guess used in these calculations.

We note that the vertical dashed lines in **Fig. S7** indicate AIMD re-starting points, which lead to sudden artificial depletions of $\langle|\mu_{\alpha C}|\rangle$. We have removed the data around such re-start times (±0.03ps) in the results presented in the main text (**Fig. 5**) to provide a clearer visualization of the physical response of the systems at finite temperatures. **Fig. S7** indicates such restart times (vertical dashed lines) plotting the raw data.

Section 3. On the on the performance of PBE0 in describing magnetic coupling in a benchmark molecular system.

In order to justify the selected hybrid DFT approach used in this work, we have analysed the electronic structure and magnetic coupling in a molecular system synthesised by Li et al.[8] for which both experimental X-ray structure and magnetic properties (from susceptibility and EPR studies) have been reported. This "superbenzene" molecular system has a ring structure of six αC centres connected via shared phenyl groups as found in TPM_{rs}. These authors reported an energy difference between the lowest singlet and triplet states of this molecule of a $\Delta E_{S\text{-}T}$ = −6.23 kcal/mol = -270 meV estimated from the temperature dependence of the intensity of EPR peaks fitted to a Bleaney-Bowers equation for a spin dimer model. Although this assumption can be questionable, the fact that the obtained energy is significantly large

justifies the simplification of the spectrum of magnetic states of this magnetic system formed by a ring of six S=1/2 coupled spins to the lowest singlet and triplet states to analyse the magnetic response of the system (i.e. the remaining singlet, triplet, quintet, and septet excited states are not thermally accessible and, hence, ignored). To relate this estimated ΔE_{S-T} energy difference with the correct Heisenberg model of the system we have to map this energy to the exact solution for an AF hexagonal Heisenberg system of S=1/2 spin particles interacting via $-2JS_iS_j$ nearest neighbour operators.[9] The exact solution for this spin model gives ΔE_{S-T} = 1.369J leading to J = -197 meV. Our calculations using unrestricted PBE0 DFT calculations within the broken-symmetry approach and employing the experimental structure provide a value of J = -249 meV. We note that the agreement with experiment is rather good considering the small energy scales involved and the uncertainty in determining accurate experimental ΔE_{S-T} values.

We can further compare this J value for the "superbenzene" molecular system for that obtained for TPM_{rs}, since it represents the magnetic coupling between two nearest neighbour αC spin centres with the same linkers and local environment. In order to do, we first need to account for the difference in the dihedral angles of the aryl rings in each system. As described previously by some of us,[10] average dihedral angles of aryl rings in play an important role in determining J values in this type of system. The average dihedral angle for unstrained TPM_{rs} is around 32-33 degrees compared to (69.1 + 2*26.6)/3 = 40.8 degrees for the experimental structure of the molecular system. Taking into account the 7-8 degrees difference in the average dihedral angle,[11] an estimated J value of -240 meV is obtained for TPM_{rs}. Note that J = -317 meV is obtained for fully relaxed TPM_{rs} with relatively flatter aryl rings (see **table S2**). The good correspondence between the J values calculated by means of our DFT calculations using the PBE0 functional for TPM_{rs} and the corresponding experimental and calculated values of the "superbenzene" molecular system provides a strong argument to support the use of the PBE0 functional to describe the electronic structure and magnetic properties of this type of system.

Section 4. Optimized geometries and single-point input files (FHI-AIMS format)

Optimized geometry for the TPM_{rs} 2D-CORF

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Optimized geometry for the PTM_{rs} 2D-CORF

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Optimized geometry for the PTM TPM$_{rs}$ 2D-CORF

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Optimized geometry for the $PTM_{acetylenic}$ 2D-CORF

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Optimized geometry for the oxTAM$_{rs}$ 2D-CORF

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atom 11.17198543 7.55035732 19.45859292 C
atom 9.77376161 7.54673589 19.45768872 C
atom 1.47921081 12.30609702 19.46550399 C
atom 7.72863603 1.54948468 19.46269419 C
atom 7.02629216 2.75860542 19.46185419 C
atom -1.26772908 7.51750545 19.46127323 C
atom -2.66607449 7.51386904 19.46064958 C
atom -0.57205450 8.73028472 19.46244519 C
atom -3.33773790 6.28110858 19.46000139 C
atom -3.34447825 8.74301782 19.46075016 C
atom -4.71862049 8.73933183 19.45922409 C
atom 0.83157697 8.70315586 19.46363365 C

```
atom     -1.30387374     9.92840873    19.46295562 C
atom     -0.62004157    11.12020742    19.46534908 C
atom      0.78364774    11.09318473    19.46588444 C
atom      1.51530116     9.89506067    19.46530103 C
atom     -1.29068871     5.10639496    19.46111811 C
atom     -0.56539324     6.30843229    19.46171837 C
atom      0.83819952     6.34309050    19.46265787 C
atom      1.52850426     5.15493951    19.46273664 C
atom     -0.60034489     3.91824675    19.46190800 C
atom     -0.59383475     1.55815896    19.46202411 C
atom      1.54157896     0.33289884    19.46282491 C
atom      4.94967543     3.98387023    19.46256528 C
atom      5.62800515     2.75464744    19.46272341 C
atom      4.95634767     1.52191517    19.46354289 C
atom      3.58217880     1.51837552    19.46351225 C
atom      3.57555558     3.98024215    19.46269711 C
atom      0.80317972     3.95288899    19.46266080 C
atom      0.80982326     1.53103514    19.46270581 C
atom      2.90386035     2.74752026    19.46305048 C
atom      1.50555447     2.74384468    19.46301024 C
atom     15.28441246     0.41027875    19.46176635 C
atom     -7.46269580    13.46210345    19.46187261 C
atom      1.52203220     7.52512200    19.46277569 O
atom      2.89407742     5.16365294    19.46314439 O
atom      5.62464606     5.17090378    19.46199525 O
atom      6.98369297     7.53930961    19.45838267 O
atom      5.61148656     9.90040182    19.46181667 O
atom      2.88084401     9.89347373    19.46589858 O
atom     -1.31049361    12.29836279    19.46606360 O
atom     -2.66947833     9.93001445    19.46131948 O
atom     -2.65623970     5.09773411    19.45886297 O
atom     -1.28423710     2.73632681    19.46207637 O
atom      2.90714647     0.33141119    19.46417854 O
atom      5.63777250     0.33853523    19.46388945 O
atom      9.81609054     2.76592424    19.46184203 O
atom     11.17512527     5.13431936    19.46066729 O
atom     -5.40022862     9.92268039    19.45839872 O
atom     -6.77234614    12.28396661    19.46159087 O
atom     11.18824434     0.40449543    19.46466973 O
atom     13.91883848     0.41190855    19.46129425 O
```

FHI-AIMS input file for single-point calculations (including basis set specification)

```
################################################################################################
#
#  ground_states
#
################################################################################################
#
#  Physical model
```

```
#
  xc               pbe0
#  spin              none
  spin             collinear
#  relativistic      none
  relativistic atomic_zora scalar
  charge           0
  default_initial_moment 0
  vdw_correction_hirshfeld
  k_grid           6 6 1
#
#  SCF convergence
#
  occupation_type    gaussian 0.01
  mixer            pulay
    n_max_pulay       10
    charge_mix_param   0.5
  sc_accuracy_rho    1E-3
  sc_accuracy_eev    1E-2
  sc_accuracy_etot   1E-5
  sc_accuracy_forces 1E-3
  sc_iter_limit      250
#
#  Relaxation
#
#  restart_relaxations .true.
#  relax_geometry   bfgs 1.e-2
#  RI_method       LVL_fast
#  relax_unit_cell   fixed_angles
# Output
#   output mulliken
   output hirshfeld_always
   output cube spin_density
#   output cube eigenstate_density  xx

# output DOS
  output dos -10. 5. 300 0.05
#dos_kgrid_factors 8 8 8

#   output band structure
  exx_band_structure_version 1
  output band   0.333333  -0.666666   0.000000   0.000000   0.000000   0.000000   100 K    G
  output band   0.000000   0.000000   0.000000  -0.333333  -0.333333   0.000000   100 G    k
  output band  -0.333333  -0.333333   0.000000   0.000000  -0.500000   0.000000   100 k    M
  output band   0.000000  -0.500000   0.000000   0.333333  -0.666666   0.000000   100 M    K


################################################################################
#
#  FHI-aims code project
#  VB, Fritz-Haber Institut, 2009
```

```
#
#  Suggested "light" defaults for C atom (to be pasted into control.in file)
#  Be sure to double-check any results obtained with these settings for post-processing,
#  e.g., with the "tight" defaults and larger basis sets.
#
################################################################################
  species       C
#     global species definitions
    nucleus           6
    mass             12.0107
#
    l_hartree         4
#
    cut_pot           3.5  1.5  1.0
    basis_dep_cutoff    1e-4
#
    radial_base       34 5.0
    radial_multiplier   1
    angular_grids specified
      division   0.3326   50
      division   0.5710  110
      division   0.7727  194
      division   0.8772  302
#       division   0.9334  434
#       division   0.9625  590
#       division   0.9924  770
#       division   1.0230  974
#       division   1.4589 1202
#     outer_grid  974
     outer_grid 302
################################################################################
#
#  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
#  "Third tier" - improvements: -2.43 meV to -0.60 meV
#    hydro 2 p 5.6
#    hydro 2 s 1.4
#    hydro 3 d 4.9
#    hydro 4 f 11.2
#  "Fourth tier" - improvements: -0.39 meV to -0.18 meV
#    hydro 2 p 2.1
#    hydro 5 g 16.4
#    hydro 4 d 13.2
#    hydro 3 s 13.6
#    hydro 4 f 17.6
#  Further basis functions - improvements: -0.08 meV and below
#    hydro 3 s 2
#    hydro 3 p 6
#    hydro 4 d 20
################################################################################
#
#  FHI-aims code project
#  VB, Fritz-Haber Institut, 2009
#
#  Suggested "light" defaults for Cl atom (to be pasted into control.in file)
#  Be sure to double-check any results obtained with these settings for post-processing,
#  e.g., with the "tight" defaults and larger basis sets.
#
################################################################################
  species       Cl
#     global species definitions
    nucleus             17
    mass                35.453
#
    l_hartree           4
#
    cut_pot             3.5         1.5  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         45 5.0
    radial_multiplier   1
    angular_grids       specified
      division   0.4412  110
      division   0.5489  194
      division   0.6734  302
#     division   0.7794  434
```

```
#     division   0.9402  590
#     division   1.0779  770
#     division   1.1792  974
#     outer_grid  974
     outer_grid  302
################################################################################
#
#  Definition of "minimal" basis
#
################################################################################
#   valence basis states
   valence     3  s   2.
   valence     3  p   5.
#   ion occupancy
   ion_occ     3  s   1.
   ion_occ     3  p   4.
################################################################################
#
#  Suggested additional basis functions. For production calculations,
#  uncomment them one after another (the most important basis functions are
#  listed first).
#
#  Constructed for dimers: 1.65 A, 2.0 A, 2.5 A, 3.25 A, 4.0 A
#
################################################################################
#  "First tier" - improvements: -429.57 meV to -15.03 meV
    ionic 3 d auto
    hydro 2 p 1.9
#    hydro 4 f 7.4
    ionic 3 s auto
#    hydro 5 g 10.4
#  "Second tier" - improvements: -7.84 meV to -0.48 meV
#    hydro 3 d 3.3
#    hydro 5 f 9.8
#    hydro 1 s 0.75
#    hydro 5 g 11.2
#    hydro 4 p 10.4
#  "Third tier" - improvements: -1.00 meV to -0.12 meV
#    hydro 4 d 12.8
#    hydro 4 f 4.6
#    hydro 4 d 10.8
#    hydro 2 s 1.8
#    hydro 3 p 3
#  Further functions that fell out - improvements: -0.10 meV and below
#    hydro 5 f 14.4
#    hydro 4 s 12.8
#    hydro 3 d 11.6
#    hydro 4 s 4.1
################################################################################
#
#  FHI-aims code project
```

```
#  VB, Fritz-Haber Institut, 2009
#
#  Suggested "light" defaults for H atom (to be pasted into control.in file)
#  Be sure to double-check any results obtained with these settings for post-processing,
#  e.g., with the "tight" defaults and larger basis sets.
#
################################################################################
 species       H
#    global species definitions
   nucleus           1
   mass              1.00794
#
   l_hartree         4
#
   cut_pot           3.5  1.5  1.0
   basis_dep_cutoff    1e-4
#
   radial_base       24 5.0
   radial_multiplier   1
   angular_grids      specified
     division   0.2421   50
     division   0.3822  110
     division   0.4799  194
     division   0.5341  302
#      division   0.5626  434
#      division   0.5922  590
#      division   0.6542  770
#      division   0.6868 1202
#      outer_grid  770
     outer_grid  302
################################################################################
#
#  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
#  "Third tier" - improvements: -0.25 meV to -0.12 meV
#     hydro 4 f 11.2
#     hydro 3 p 4.8
#     hydro 4 d 9
#     hydro 3 s 3.2
################################################################################
#
#  FHI-aims code project
#  VB, Fritz-Haber Institut, 2009
#
#  Suggested "light" defaults for O atom (to be pasted into control.in file)
#  Be sure to double-check any results obtained with these settings for post-processing,
#  e.g., with the "tight" defaults and larger basis sets.
#
################################################################################
  species       O
#     global species definitions
    nucleus             8
    mass               15.9994
#
    l_hartree           4
#
    cut_pot             3.5  1.5  1.0
    basis_dep_cutoff    1e-4
#
    radial_base         36 5.0
    radial_multiplier   1
     angular_grids specified
      division   0.2659   50
      division   0.4451  110
      division   0.6052  194
      division   0.7543  302
#     division   0.8014  434
#     division   0.8507  590
#     division   0.8762  770
#     division   0.9023  974
#     division   1.2339 1202
#     outer_grid 974
      outer_grid 302
################################################################################
#
#  Definition of "minimal" basis
#
################################################################################
#     valence basis states
    valence      2  s   2.
```

```
   valence     2  p   4.
#    ion occupancy
   ion_occ     2  s   1.
   ion_occ     2  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: 1.0 A, 1.208 A, 1.5 A, 2.0 A, 3.0 A
#
#############################################################################
#  "First tier" - improvements: -699.05 meV to -159.38 meV
    hydro 2 p 1.8
    hydro 3 d 7.6
    hydro 3 s 6.4
#  "Second tier" - improvements: -49.91 meV to -5.39 meV
#    hydro 4 f 11.6
#    hydro 3 p 6.2
#    hydro 3 d 5.6
#    hydro 5 g 17.6
#    hydro 1 s 0.75
#  "Third tier" - improvements: -2.83 meV to -0.50 meV
#    ionic 2 p auto
#    hydro 4 f 10.8
#    hydro 4 d 4.7
#    hydro 2 s 6.8
#  "Fourth tier" - improvements: -0.40 meV to -0.12 meV
#    hydro 3 p 5
#    hydro 3 s 3.3
#    hydro 5 g 15.6
#    hydro 4 f 17.6
#    hydro 4 d 14
# Further basis functions - -0.08 meV and below
#    hydro 3 s 2.1
#    hydro 4 d 11.6
#    hydro 3 p 16
#    hydro 2 s 17.2
```

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