Cyclo[*n*]carbons and catenanes from different perspective. Disentangling molecular thread

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Supporting Information

Table S1 Evolution of in-plane NICS along the stretching of the $2xC_{18}$ thread. Definition of Bq centres is in Figure S3.

$R_{ij,max}$ [Å]	Strain [%]	$C_{left,outer}$	$C_{left,inner}$	$C_{right,inner}$	$C_{right,outer}$
11.004	7.4	-30.750	-45.910	-45.910	-30.751
12.366	14.9	-32.837	-46.210	-46.197	-32.786
13.166	22.3	-33.390	-44.854	-44.866	-33.372
13.966	29.7	-33.438	-42.464	-42.421	-33.373
14.665	36.2	-33.016	-42.653	-42.689	-32.966
15.365	42.7	-32.348	-34.537	-34.536	-32.305
16.000	48.6	-25.111	-34.823	-34.836	-27.114
16.761	55.7	-19.736	-20.196	-19.863	-15.859
17.360	61.2	-15.727	0.010	0.491	-13.278

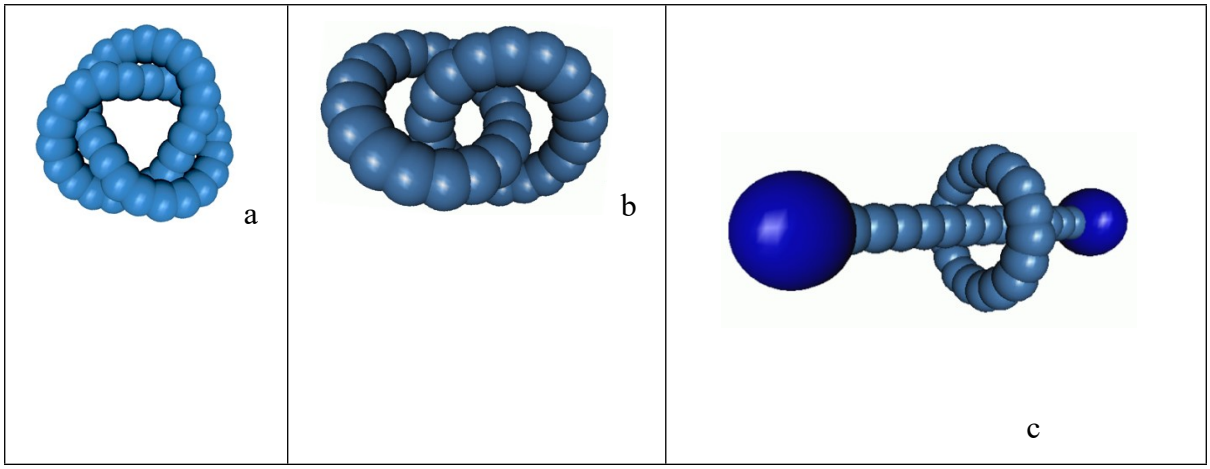
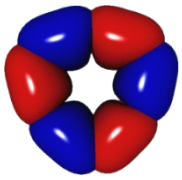
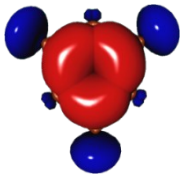
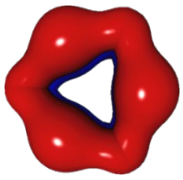
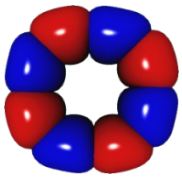
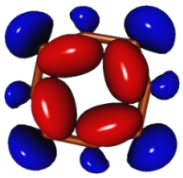
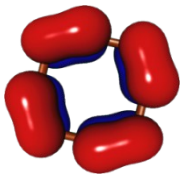
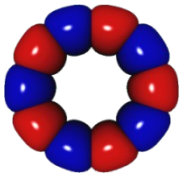
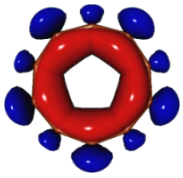
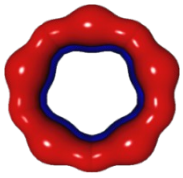
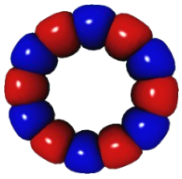
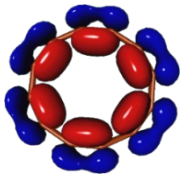
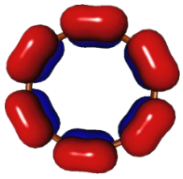
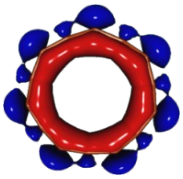
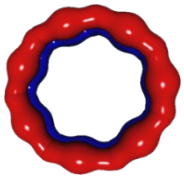
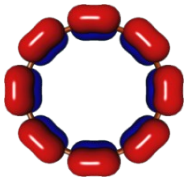
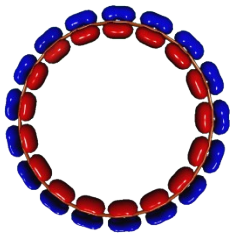


Figure S1. Three examples of mechanically interlocked molecules (MIMs): a) knot; b) catenane; c) rotaxane.

C_n	Results of AdNDP analysis		
	σ orbitals	**π orbitals in plane**	**π orbitals out of plane**
C_6			
C_8			
C_{10}			
C_{12}			

C_{14}			
C_{16}			
C_{18}			
C_{20}			
C_{22}			
C_{24}			
C_{26}			

C_{28}			
C_{30}			
C_{32}			
C_{34}			
C_{36}			
C_{38}			
C_{40}			

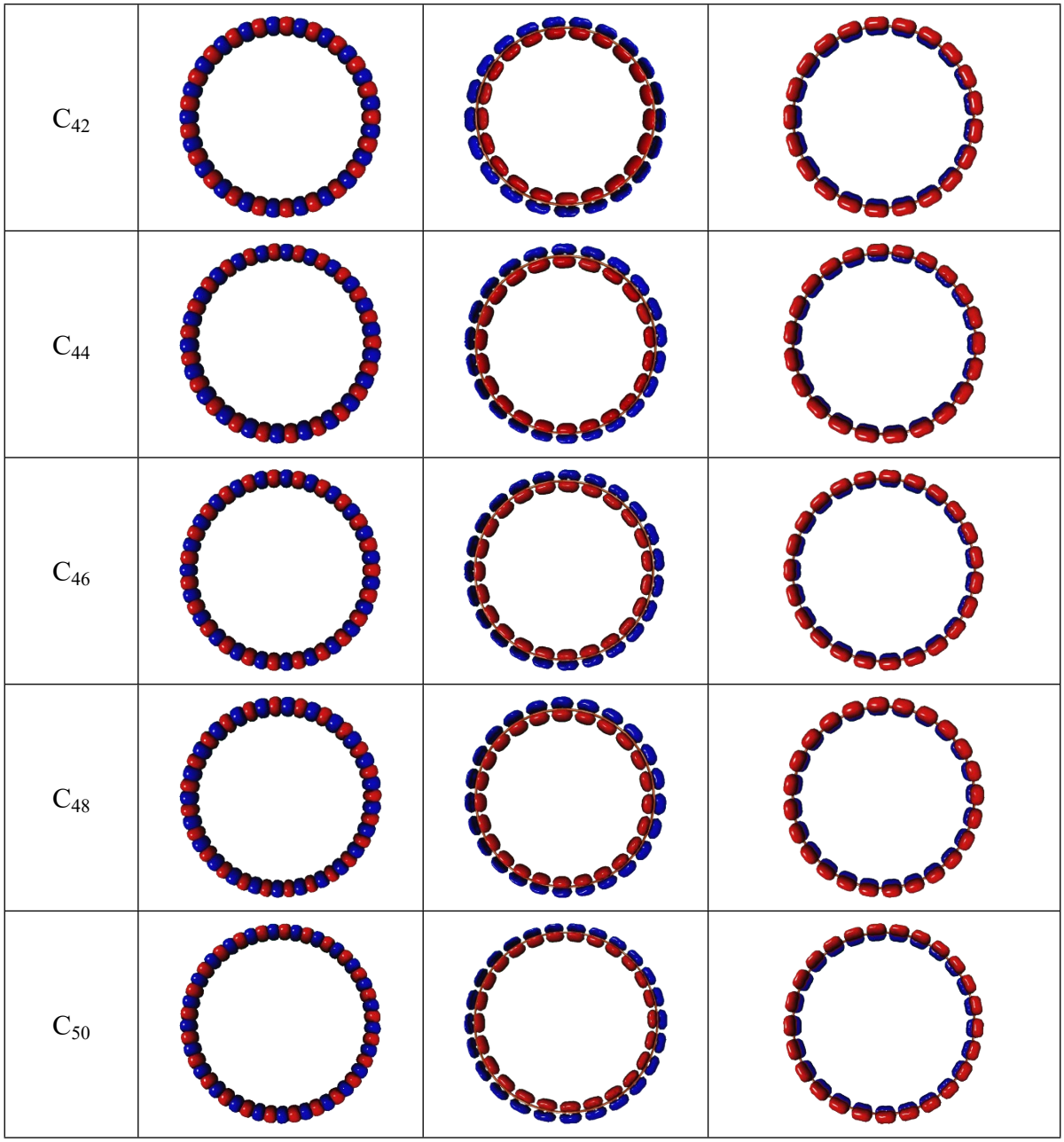


Figure S2. Complete gallery of AdNDP analysis for cyclo[*n*]carbons, *n* = 6 – 50, from geometries optimized at ωB97XD/6-31+G* level – orbitals σ and π orbitals (in and out of plane). Contour value 0.1 was adopted for each picture.

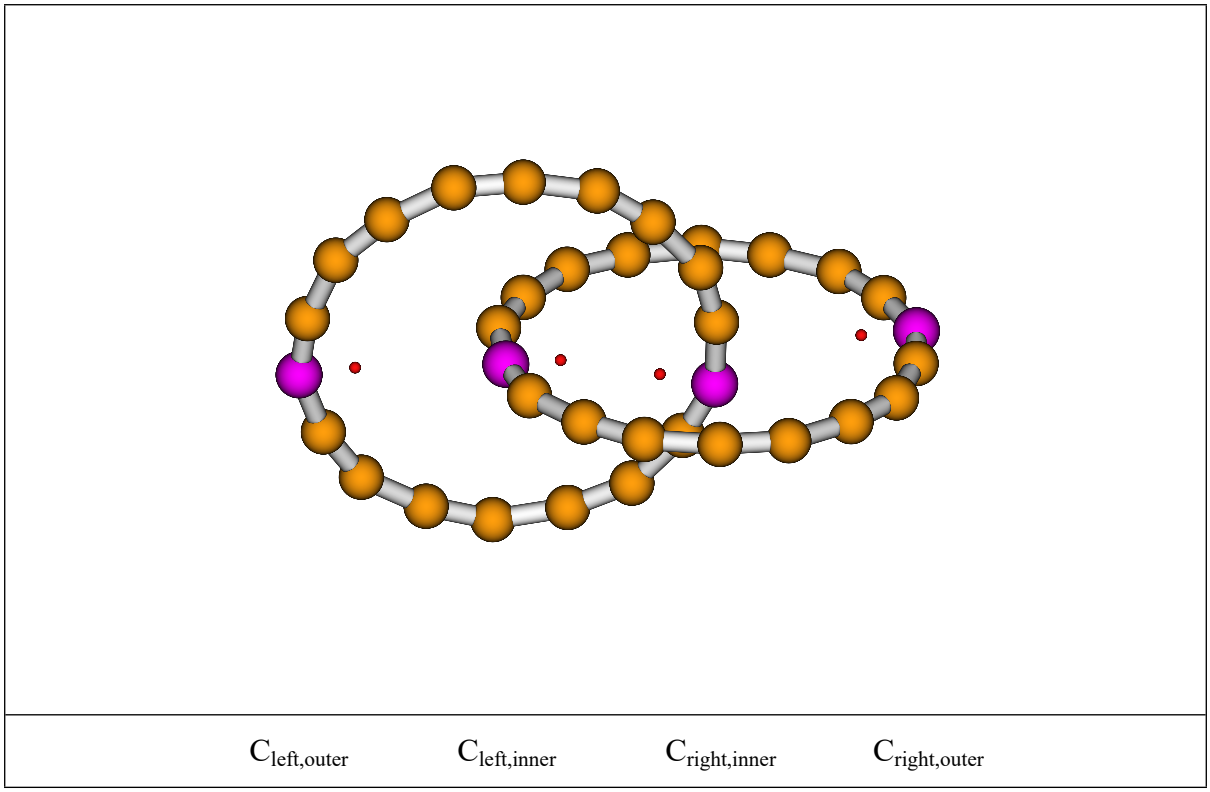


Figure S3. Definition of Bq centers (red dots) lying in the ring plane and adjacent to peripheral carbon atoms (magenta circles) for model catenane $2xC_{18}$.