

-- Supporting Information For --
**Switch from Local to Global Aromatic Character
in Möbius Carbon Nanobelts upon Dioxidation.
Evaluation of Magnetic Behavior in Neutral and
Charged species**

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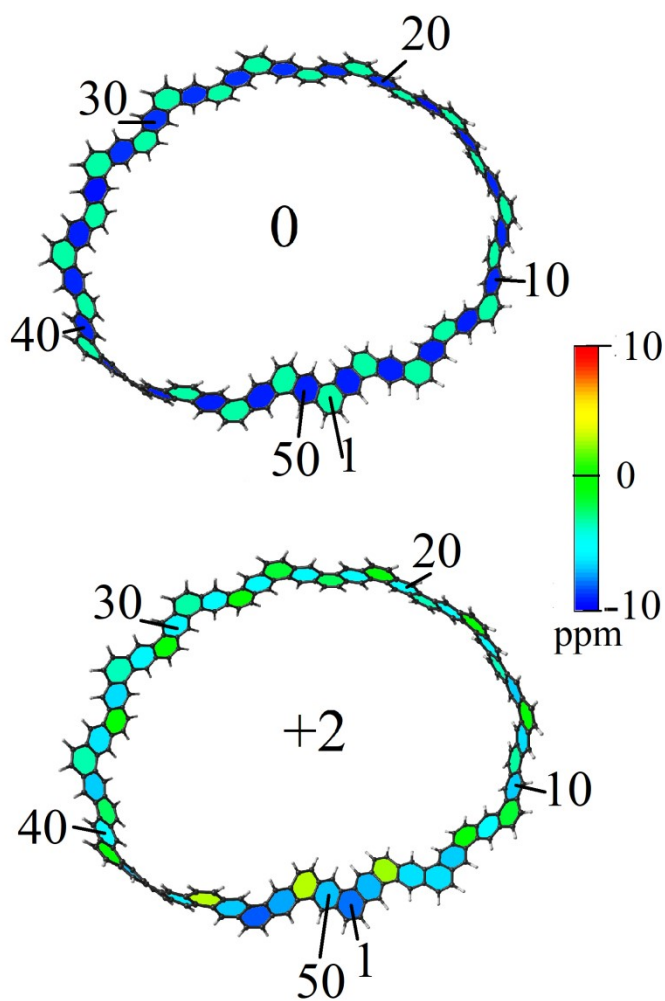
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Table S1. NICS values at the center of each fused benzene ring. Values in ppm.

Ring N°	0	2+
1	-2.94	-7.91
2	-9.11	-6.56
3	-3.00	3.57
4	-9.46	-5.46
5	-2.96	-5.55
6	-9.29	-5.95
7	-2.82	0.17
8	-9.46	-5.14
9	-3.13	-1.91
10	-9.33	-5.73
11	-3.02	-3.05
12	-9.36	-5.39
13	-3.01	0.14
14	-9.37	-5.39
15	-2.98	-3.78
16	-9.35	-5.26
17	-3.04	0.55
18	-9.50	-5.18
19	-3.05	-3.16
20	-9.41	-5.22
21	-2.99	-0.29
22	-9.47	-4.94
23	-2.98	-1.62
24	-9.41	-5.18
25	-2.97	-1.74
26	-9.46	-4.96
27	-3.00	-0.26
28	-9.40	-5.26
29	-3.03	-3.27
30	-9.45	-5.22
31	-3.07	0.53
32	-9.37	-5.27
33	-2.98	-3.75
34	-9.37	-5.40
35	-3.05	0.12
36	-9.35	-5.34
37	-3.05	-3.11
38	-9.36	-5.72
39	-3.22	-1.98
40	-9.38	-5.11
41	-2.87	0.28
42	-9.27	-5.99
43	-2.93	-5.54
44	-9.23	-5.50



45	-2.86	3.48
46	-9.06	-6.60
47	-2.94	-8.15
48	-9.14	-6.98
49	-2.99	4.02
50	-9.12	-6.67

Table S2. NICS values at the center of each fused benzene ring, at different levels of theory involving PBE0/TZ2P, CAM-B3LYP/TZ2P and M06-2X/TZ2P. Values in ppm. Numeration given on Table S1 schematic.

Ring N°	PBE0		CAM-B3LYP		M06-2X	
	0	2+	0	2+	0	2+
1	-2.94	-7.91	-3.42	-8.92	-10.64	-32.28
2	-9.11	-6.56	-10.61	-7.39	-32.98	-26.77
3	-3.00	3.57	-3.49	4.02	-10.86	14.57
4	-9.46	-5.46	-11.02	-6.15	-34.25	-22.28
5	-2.96	-5.55	-3.45	-6.26	-10.72	-22.65
6	-9.29	-5.95	-10.82	-6.71	-33.63	-24.28
7	-2.82	0.17	-3.28	0.19	-10.21	0.69
8	-9.46	-5.14	-11.02	-5.79	-34.25	-20.98
9	-3.13	-1.91	-3.65	-2.15	-11.33	-7.79
10	-9.33	-5.73	-10.87	-6.46	-33.78	-23.38
11	-3.02	-3.05	-3.52	-3.44	-10.93	-12.45
12	-9.36	-5.39	-10.90	-6.08	-33.89	-22.00
13	-3.01	0.14	-3.51	0.16	-10.90	0.57
14	-9.37	-5.39	-10.91	-6.08	-33.92	-22.00
15	-2.98	-3.78	-3.47	-4.26	-10.79	-15.43
16	-9.35	-5.26	-10.89	-5.93	-33.85	-21.47
17	-3.04	0.55	-3.54	0.62	-11.01	2.24
18	-9.50	-5.18	-11.07	-5.84	-34.39	-21.14
19	-3.05	-3.16	-3.55	-3.56	-11.04	-12.90
20	-9.41	-5.22	-10.96	-5.88	-34.07	-21.30
21	-2.99	-0.29	-3.48	-0.33	-10.83	-1.18
22	-9.47	-4.94	-11.03	-5.57	-34.29	-20.16
23	-2.98	-1.62	-3.47	-1.83	-10.79	-6.61
24	-9.41	-5.18	-10.96	-5.84	-34.07	-21.14
25	-2.97	-1.74	-3.46	-1.96	-10.75	-7.10
26	-9.46	-4.96	-11.02	-5.59	-34.25	-20.24
27	-3.00	-0.26	-3.49	-0.29	-10.86	-1.06
28	-9.40	-5.26	-10.95	-5.93	-34.03	-21.47
29	-3.03	-3.27	-3.53	-3.69	-10.97	-13.34
30	-9.45	-5.22	-11.01	-5.88	-34.21	-21.30
31	-3.07	0.53	-3.58	0.60	-11.11	2.16
32	-9.37	-5.27	-10.91	-5.94	-33.92	-21.51
33	-2.98	-3.75	-3.47	-4.23	-10.79	-15.30

34	-9.37	-5.40	-10.91	-6.09	-33.92	-22.04
35	-3.05	0.12	-3.55	0.14	-11.04	0.49
36	-9.35	-5.34	-10.89	-6.02	-33.85	-21.79
37	-3.05	-3.11	-3.55	-3.51	-11.04	-12.69
38	-9.36	-5.72	-10.90	-6.45	-33.89	-23.34
39	-3.22	-1.98	-3.75	-2.23	-11.66	-8.08
40	-9.38	-5.11	-10.93	-5.76	-33.96	-20.85
41	-2.87	0.28	-3.34	0.32	-10.39	1.14
42	-9.27	-5.99	-10.80	-6.75	-33.56	-24.45
43	-2.93	-5.54	-3.41	-6.24	-10.61	-22.61
44	-9.23	-5.50	-10.75	-6.20	-33.42	-22.45
45	-2.86	3.48	-3.33	3.92	-10.35	14.20
46	-9.06	-6.60	-10.55	-7.44	-32.80	-26.93
47	-2.94	-8.15	-3.42	-9.19	-10.64	-33.26
48	-9.14	-6.98	-10.65	-7.87	-33.09	-28.49
49	-2.99	4.02	-3.48	4.53	-10.83	16.41
50	-9.12	-6.67	-10.62	-7.52	-33.02	-27.22

Figure S1. Calculated $^1\text{H-NMR}$ values referenced to C_6H_6 in CDCl_3 (7.36 ppm).

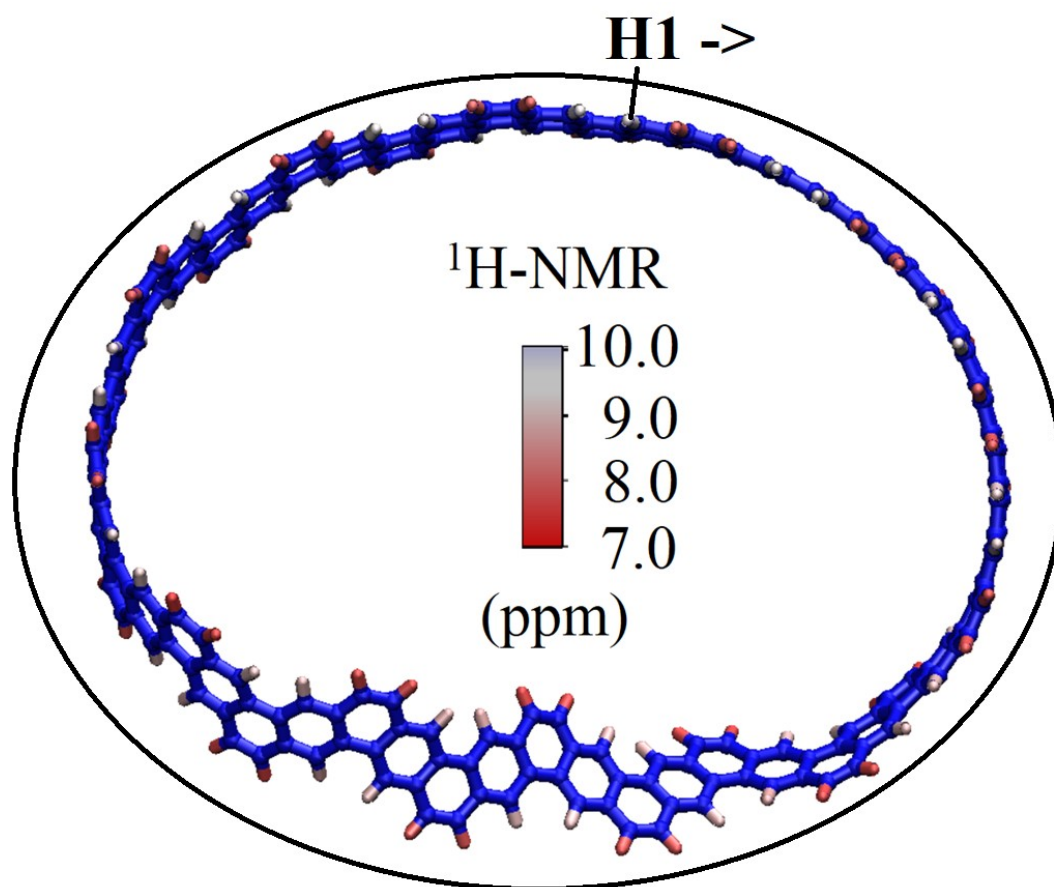


Table S3. Calculated $^1\text{H-NMR}$ values referenced to C_6H_6 in CDCl_3 (7.36 ppm)

H1	9.3	H19	7.9	H37	8.9	H55	7.8	H73	9.1	H91	9.2
H2	8.0	H20	9.2	H38	7.7	H56	8.8	H74	7.8	H92	7.9
H3	8.0	H21	9.1	H39	8.9	H57	8.8	H75	9.0	H93	9.3
H4	9.3	H22	7.9	H40	7.7	H58	7.7	H76	7.8	H94	7.9
H5	9.2	H23	9.1	H41	8.8	H59	8.7	H77	9.1	H95	7.9
H6	7.9	H24	7.8	H42	7.7	H60	7.7	H78	7.9	H96	9.2
H7	9.3	H25	9.0	H43	7.7	H61	8.9	H79	7.8	H97	9.3
H8	7.9	H26	7.7	H44	8.8	H62	7.7	H80	9.1	H98	8.0
H9	9.2	H27	7.8	H45	8.8	H63	7.7	H81	9.2	H99	9.3
H10	7.8	H28	9.1	H46	7.8	H64	9.0	H82	7.8	H100	8.0
H11	7.9	H29	9.1	H47	8.7	H65	8.9	H83	9.2		
H12	9.2	H30	7.8	H48	7.8	H66	7.7	H84	7.9		
H13	9.2	H31	9.0	H49	8.9	H67	8.9	H85	9.2		
H14	8.0	H32	7.8	H50	7.7	H68	7.6	H86	8.0		
H15	9.2	H33	8.9	H51	8.9	H69	9.0	H87	7.9		
H16	7.9	H34	7.7	H52	7.7	H70	7.8	H88	9.2		
H17	9.2	H35	7.6	H53	8.8	H71	7.8	H89	9.2		
H18	7.8	H36	8.8	H54	7.8	H72	9.1	H90	7.8		

Table S4. Coordinates for optimized geometries. Values in Å.

300

(25, 25)MCNB q=0

C	1.422887041	0.231239419	-14.866026286
C	0.510881803	1.290057783	-14.912455256
C	1.777455769	-2.217337236	-14.942652258
C	0.880992858	-1.095706606	-14.917822849
C	-0.510881803	-1.290057783	-14.912455256
C	-1.422887041	-0.231239419	-14.866026286
C	-0.880992858	1.095706606	-14.917822849
C	-3.124421342	2.054922001	-14.846153675
C	-1.777455769	2.217337236	-14.942652258
C	-3.488733599	-1.642987999	-14.525508119
C	-2.870735452	-0.403977897	-14.718944343
C	-5.091358799	0.621102957	-14.443688156
C	-3.714451334	0.755198536	-14.689058217
C	-5.428159115	-3.061658709	-13.962093541
C	-4.859974968	-1.774199688	-14.248318070
C	-7.098273369	-0.761665410	-13.781644311
C	-5.697683842	-0.612209033	-14.186052778
C	-7.999041370	0.302977375	-13.687799245
C	-6.717773300	-3.195028203	-13.549307675
C	-8.872828083	-2.199044473	-12.862592882
C	-7.582415523	-2.057819395	-13.403244144
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C	-9.291674955	0.160348422	-13.156454973
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C	-14.797353796	-2.379946890	-8.651980599
C	-16.411783056	-1.196010979	-7.220930639
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C	-17.652949619	1.285037775	-6.567279333
C	-16.898583775	1.185567994	-7.694361330
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C	-18.095082635	-3.035193184	-2.899458585
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C	-18.478446670	-2.827746516	-1.610365211
C	-19.001505386	-1.279089442	0.243206080
C	-18.820745280	-1.517688568	-1.130227304
C	-19.224626882	0.000000000	0.764026350
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C	-19.635170027	2.398013060	0.297056766
C	-18.958976448	-0.624371786	3.203401063
C	-19.164295458	0.321428886	2.192777823
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C	-17.562241537	2.775131131	6.511319299
C	-17.909944079	-0.929408057	6.754752968
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C	-16.220818672	4.383519330	7.804276371

C	-14.919531641	1.387158935	10.511844516
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C	-13.504505730	3.763077606	10.251620212
C	-14.677870854	3.569557608	9.506490707
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C	-12.976645650	2.773660039	11.084537825
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C	-9.307208472	3.591236661	11.594216925
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C	8.920856840	-2.632640616	12.588817376
C	7.496637489	-2.458337922	12.887639291
C	9.925236645	-1.807482699	13.107921556
C	8.294834804	-4.321778887	10.885540218
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C	11.639677955	-2.831674556	11.673720483
C	11.250335688	-1.843126274	12.634723518
C	13.377140968	-0.682388446	12.328888808
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C	13.782075294	-1.610143036	11.308842250
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C	16.755336261	-3.062346814	7.622849607
C	17.943821080	-1.473213395	6.174484666
C	17.588407293	-0.430142325	7.091235846
C	18.400240093	1.260081575	5.528923608
C	17.909944079	0.929408057	6.754752968
C	18.907969174	-2.059064147	3.915029541
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C	19.223948615	-1.696967486	2.595651359
C	19.224626882	0.000000000	0.764026350
C	19.164295458	-0.321428886	2.192777823
C	19.001505386	1.279089442	0.243206080
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C	18.479958640	0.655101013	-3.451125374
C	17.419407845	2.139098612	-5.101726593
C	18.015347942	1.954168860	-3.842175921
C	17.652949619	-1.285037775	-6.567279333
C	17.792920859	-0.181559836	-5.658897986
C	16.411783056	1.196010979	-7.220930639
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C	15.734726500	2.358168421	-7.604763504
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C	15.281923906	0.054435469	-9.085819989
C	16.204754247	0.027066236	-8.026739279
C	14.515794372	1.183667682	-9.391078377
C	14.797353796	2.379946890	-8.651980599
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