

# Journal Name

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Electronic Supplementary Information

### The magnetically induced current density of the [12]infinetene dianion<sup>†</sup>

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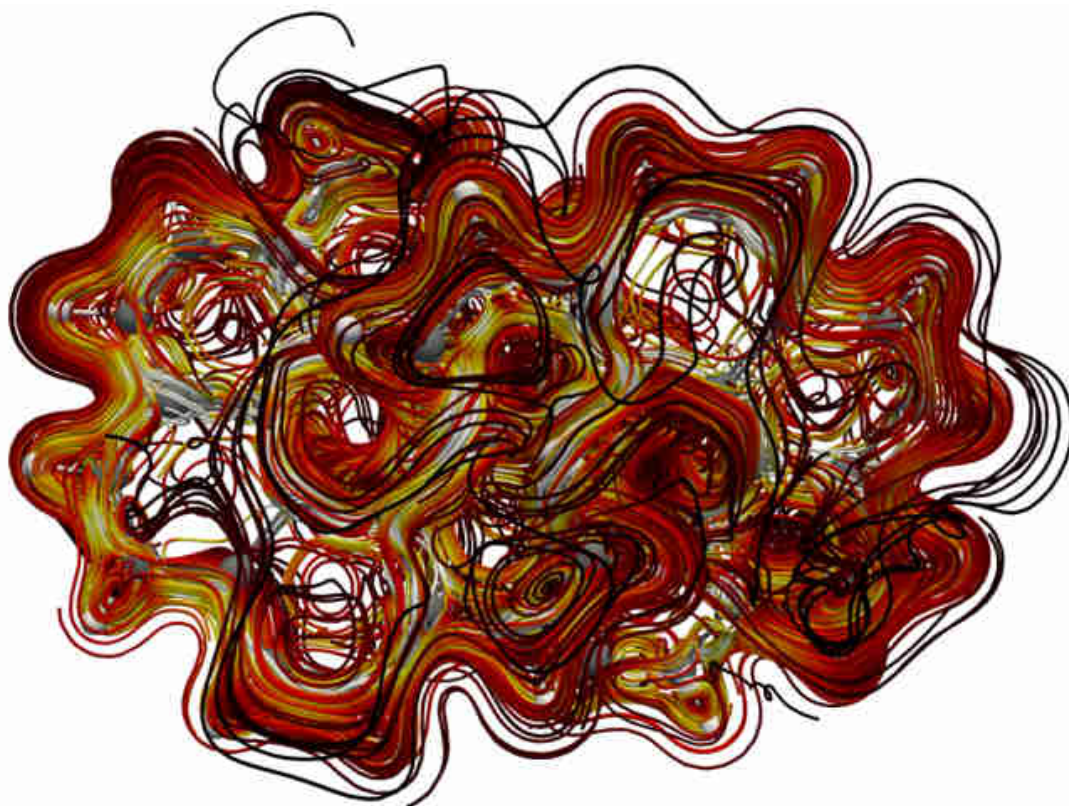
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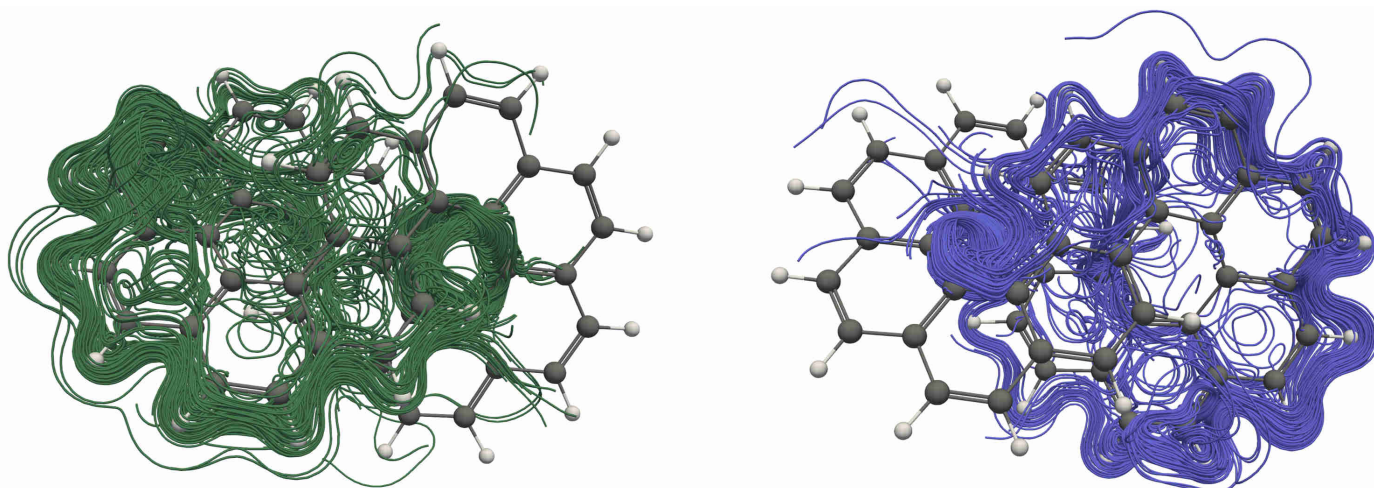
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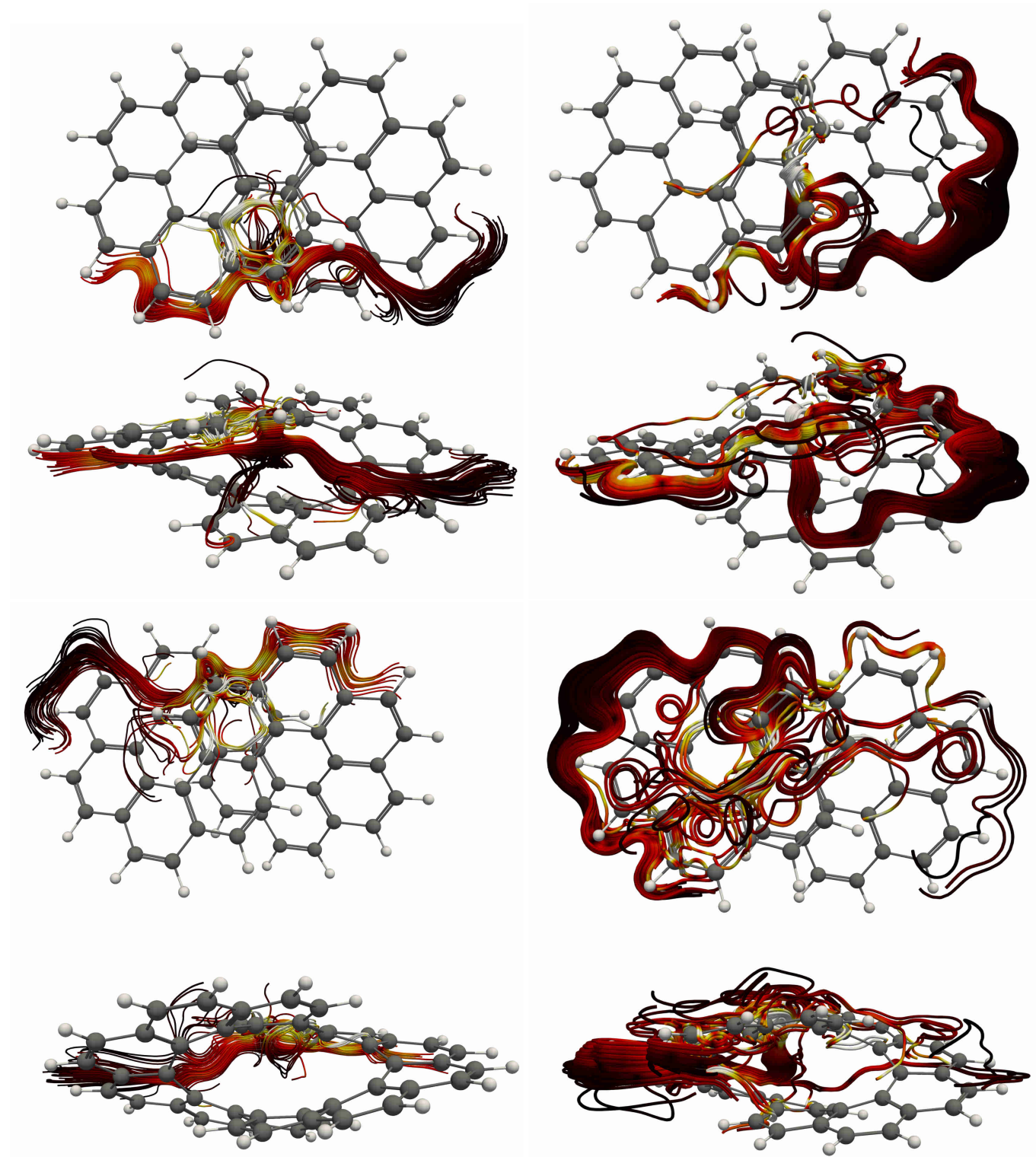
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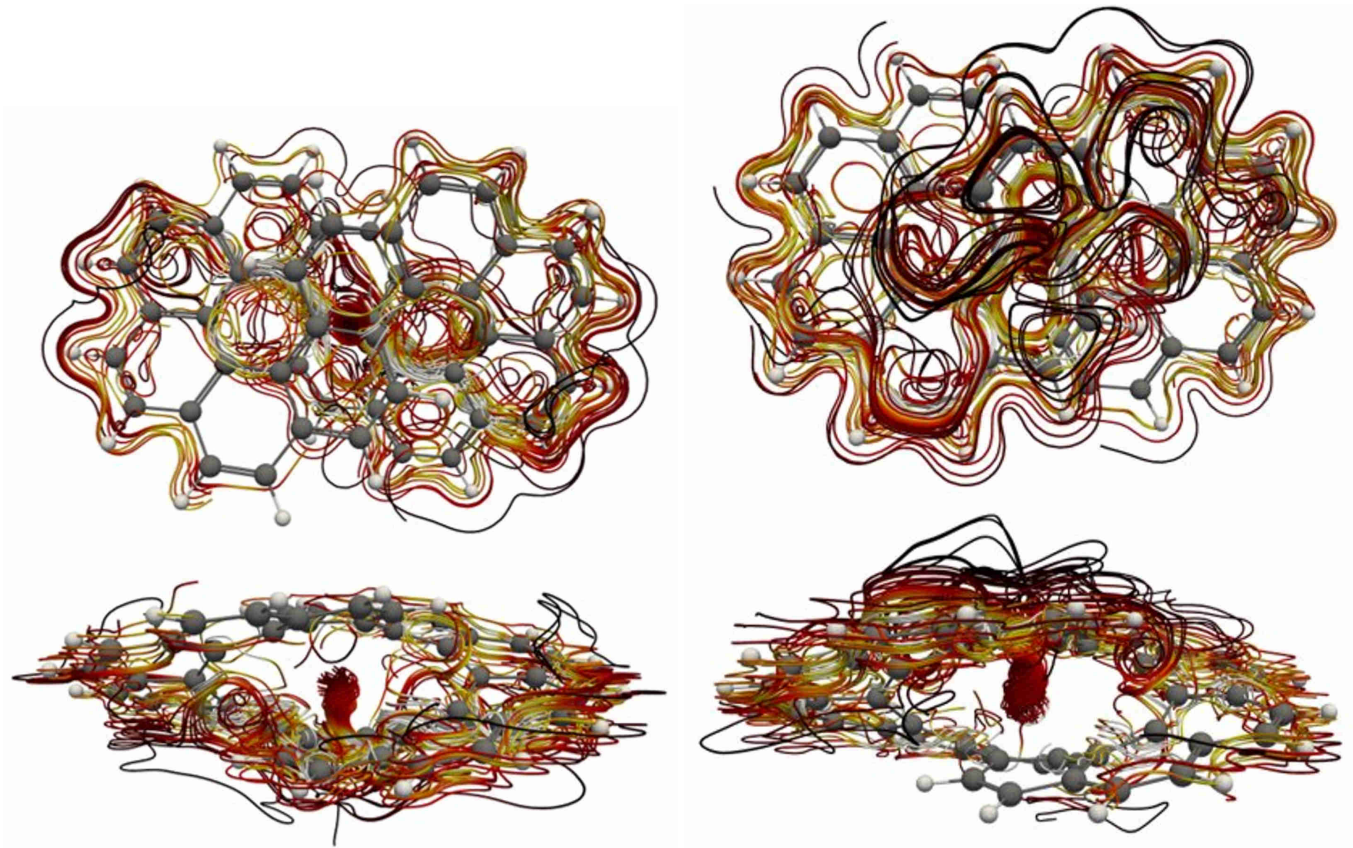
**Figure S1** The current density of [12]annulene dianion. The color scheme corresponds to the strength of the current density with white being the strongest and then yellow and then red, the weakest ones are black. The pictures have been made with Paraview.



**Figure S2** Two independent global ring currents are shown in green and blue, respectively. The current-density pictures have been made with paraview.



**Figure S3** The current density through the space from one side of the molecule to the other. The color scheme corresponds to the strength of the current density with white being the strongest and then yellow and then red, the weakest ones are black. The current-density pictures have been made with paraview.



**Figure S4** Through-space current-density pathways. The color scheme corresponds to the strength of the current density with white being the strongest and then yellow and then red, the weakest ones are black. The current-density pictures have been made with paraview.

Cartesian coordinates (in Å) of the optimized molecular structure of the [12]infinite dianion

C	-1.2395717	-1.3322532	-1.7254663
C	-0.4129834	-2.4350223	-1.8916262
C	0.9495472	-2.3475613	-1.6173251
C	1.7470821	-3.5242295	-1.6477682
C	3.0550517	-3.4721249	-1.3370063
C	3.6609789	-2.2619821	-0.8879886
C	5.0481637	-2.2588918	-0.6974232
C	5.6990163	-1.1094940	-0.3501065
C	4.9582058	0.0263987	0.0137249
C	5.6843758	1.1796269	0.4058729
C	5.0397639	2.2890878	0.8188774
C	3.6333894	2.2717276	1.0083783
C	2.8841475	1.0887989	0.7611581
C	3.5271613	0.0230814	0.0315929
C	2.8674652	-1.0829585	-0.7054509
C	1.5490186	-1.1014397	-1.2431133
C	0.7164399	0.0807380	-1.4596414
C	1.2395717	1.3322532	-1.7254663
C	-0.7164399	-0.0807380	-1.4596414
C	0.4129834	2.4350223	-1.8916262
C	-1.5490186	1.1014397	-1.2431133
C	-0.9495472	2.3475613	-1.6173251
C	-2.8674652	1.0829585	-0.7054509
C	-1.7470821	3.5242295	-1.6477682
C	-3.6609789	2.2619821	-0.8879886
C	-3.5271613	-0.0230814	0.0315929
C	-3.0550517	3.4721249	-1.3370063
C	-5.0481637	2.2588918	-0.6974232
C	-4.9582058	-0.0263987	0.0137249
C	-2.8841475	-1.0887989	0.7611581
C	-5.6990163	1.1094940	-0.3501065
C	-5.6843758	-1.1796269	0.4058729
C	-3.6333894	-2.2717276	1.0083783
C	-1.4955177	-1.1159206	1.2127460
C	-5.0397639	-2.2890878	0.8188774
C	-3.0093782	-3.4737765	1.4170972
C	-0.8842092	-2.3740475	1.4915577
C	-1.6596043	-3.5393660	1.5789862
C	-0.7073152	0.0472485	1.4303657
C	0.7073152	-0.0472485	1.4303657
C	3.0093782	3.4737765	1.4170972
C	1.2834080	-1.3321509	1.6396071
C	0.5043606	-2.4359837	1.7378887
C	1.4955177	1.1159206	1.2127460
C	-0.5043606	2.4359837	1.7378887
C	-1.2834080	1.3321509	1.6396071
C	1.6596043	3.5393660	1.5789862
C	0.8842092	2.3740475	1.4915577
H	-0.8318396	-3.4044851	-2.1316553
H	1.2803754	-4.4577393	-1.9414524
H	3.6805167	-4.3545247	-1.4123315
H	5.5975335	-3.1724578	-0.8929414
H	6.7799862	-1.0638162	-0.3060477
H	6.7656205	1.1516944	0.3414843

H	5.5818112	3.1969745	1.0553773
H	0.8318396	3.4044851	-2.1316553
H	-1.2803754	4.4577393	-1.9414524
H	-3.6805167	4.3545247	-1.4123315
H	-5.5975335	3.1724578	-0.8929414
H	-6.7799862	1.0638162	-0.3060477
H	-6.7656205	-1.1516944	0.3414843
H	-5.5818112	-3.1969745	1.0553773
H	-3.6300294	-4.3522503	1.5460751
H	-1.1698175	-4.4771577	1.8136873
H	2.3104936	1.4574735	-1.7946905
H	-2.3104936	-1.4574735	-1.7946905
H	2.3516338	-1.4081383	1.7737066
H	0.9433626	-3.4003219	1.9638511
H	-2.3516338	1.4081383	1.7737066
H	3.6300294	4.3522503	1.5460751
H	1.1698175	4.4771577	1.8136873
H	-0.9433626	3.4003219	1.9638511

The  $^1\text{H}$  NMR shielding constants of [12]infinite dianion

No.	Type	Mult.	Isotropic
49	h	2	27.39803128
50	h	2	25.90574235
51	h	2	24.84621133
52	h	2	24.67419763
53	h	2	24.55579936
54	h	2	23.65424114
55	h	2	23.84713488
56	h	0	27.39803128
57	h	0	25.90574235
58	h	0	24.84621133
59	h	0	24.67419763
60	h	0	24.55579936
61	h	0	23.65424114
62	h	0	23.84713488
63	h	2	24.26090419
64	h	2	24.14512372
65	h	2	33.75926338
66	h	0	33.75926338
67	h	2	30.75342136
68	h	2	24.90513054
69	h	0	30.75342136
70	h	0	24.26090419
71	h	0	24.14512372
72	h	0	24.90513054

The  $^{13}\text{C}$  NMR shielding constants of [12]infinite dianion

1	c	2	55.15964391
2	c	2	71.86258635
3	c	2	31.11896143
4	c	2	54.19760558
5	c	2	54.26224097
6	c	2	35.46318305
7	c	2	67.33901553
8	c	2	74.13565009
9	c	2	34.98442954

10	c	2	52.64918584
11	c	2	58.26958449
12	c	2	36.91836590
13	c	2	52.84282709
14	c	2	72.13481456
15	c	2	45.24510831
16	c	2	67.30673418
17	c	2	58.59759910
18	c	0	55.15964391
19	c	0	58.59759910
20	c	0	71.86258635
21	c	0	67.30673418
22	c	0	31.11896143
23	c	0	45.24510831
24	c	0	54.19760558
25	c	0	35.46318305
26	c	0	72.13481456
27	c	0	54.26224097
28	c	0	67.33901553
29	c	0	34.98442954
30	c	0	52.84282709
31	c	0	74.13565009
32	c	0	52.64918584
33	c	0	36.91836590
34	c	2	71.67819259
35	c	0	58.26958449
36	c	2	66.44645264
37	c	2	51.53876124
38	c	2	56.33880687
39	c	2	46.20077831
40	c	0	46.20077831
41	c	0	66.44645264
42	c	2	51.16001659
43	c	2	52.72499869
44	c	0	71.67819259
45	c	0	52.72499869
46	c	0	51.16001659
47	c	0	56.33880687
48	c	0	51.53876124

## NMR chemical shifts

### <sup>1</sup>H NMR (in ppm) of the [12]infinite dianion

<sup>1</sup>H NMR (in ppm) for atoms close to the holes in [12]infinite dianion

The TMS reference shielding constant 31.89235531 ppm

Shielding constant	Chemical shift
33.75926338	-1.86690807
30.75342136	1.13893395

<sup>1</sup>H NMR (in ppm) for atoms far away from the holes in [12]infinite dianion

The TMS reference shielding constant 31.89235531 ppm

Shielding constant	Chemical shift
27.39803128	4.49432403
25.90574235	5.98661296
24.84621133	7.04614398
24.67419763	7.21815768
24.55579936	7.33655595

23.65424114	8.23811417
23.84713488	8.04522043
24.26090419	7.63145112
24.14512372	7.74723159
24.90513054	6.98722477

**<sup>13</sup>C NMR (in ppm) of the [12]infinite dianion**

The TMS reference shielding constant 188.54716189 ppm

Shielding constant	Chemical shift
55.15964391	133.38751798
71.86258635	116.68457554
31.11896143	157.42820046
54.19760558	134.34955631
54.26224097	134.28492092
35.46318305	153.08397884
67.33901553	121.20814636
74.13565009	114.41151180
34.98442954	153.56273235
52.64918584	135.89797605
58.26958449	130.27757740
36.91836590	151.62879599
52.84282709	135.70433480
72.13481456	116.41234733
45.24510831	143.30205358
67.30673418	121.24042771
58.59759910	129.94956279
71.67819259	116.86896930
66.44645264	122.10070925
51.53876124	137.00840065
56.33880687	132.20835502
46.20077831	142.34638358
51.16001659	137.38714530
52.72499869	135.82216320