

The aromatic character of [10]annulenes and dicupra[10]annulenes from current density calculations

Maria Dimitrova^a and Dage Sundholm^a

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^a University of Helsinki, Department of Chemistry, P.O. Box 55, A. I. Virtasen aukio 1, FIN-00014 University of Helsinki, Finland and Centre for Advanced Study at the Norwegian Academy of Science and Letters, Drammensveien 78, N-0271 Oslo, Norway. E- mail: maria.dimitrova@helsinki.fi, dage.sundholm@helsinki.fi

1 Current profile plots

1.1 Naphthalene

Current profile plots and integrated domains in the plots (in nA/T). The origin on the abscissa lies at the beginning of the integration plane, which lies at the centre of a ring unless otherwise noted.

Table 1 Plane a with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-2.31	10.69	20.32
0.01	10.69	12.60
Diatropic domains		
-2.31	0.01	7.74
0.01	10.69	17.61
Paratropic domains		
-0.11	2.29	-4.98

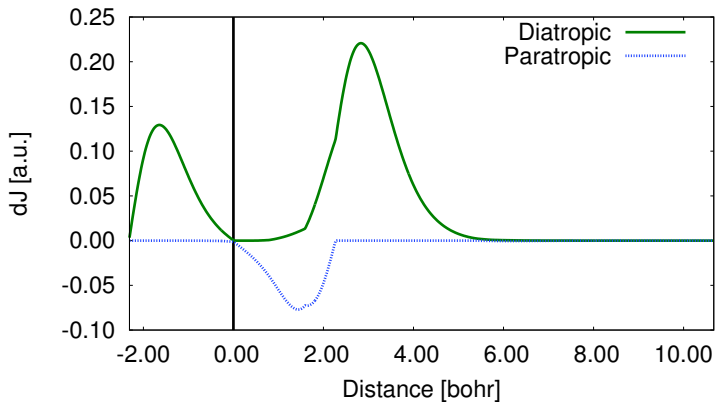


Table 2 Plane b with origin at the midpoint of the bond C5 – C10 and continuing along the bond to infinity.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	13.34	21.18
Diatropic domains		
-0.04	13.34	30.47
Paratropic domains		
1.00	1.34	-9.13

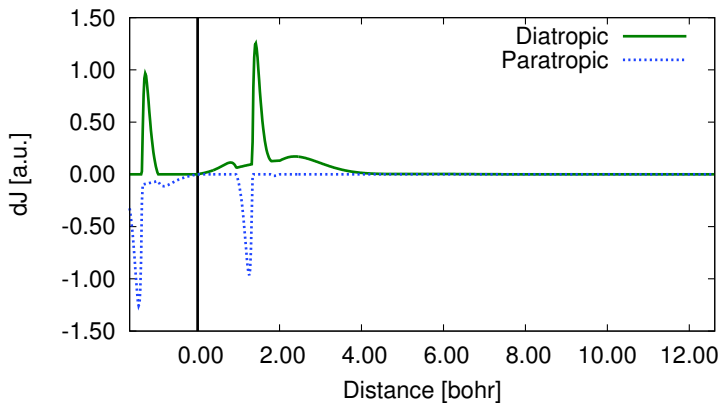
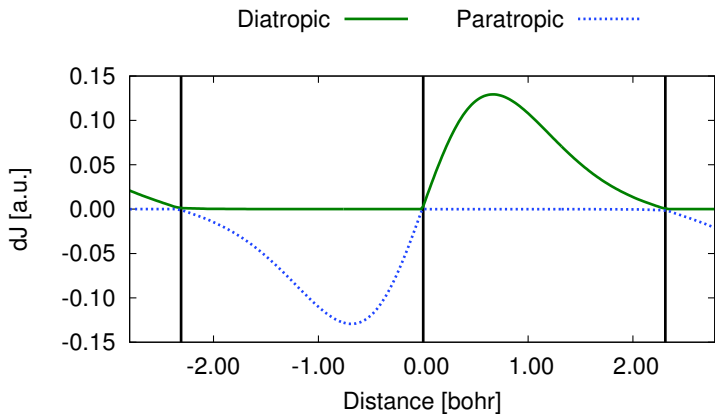


Table 3 Plane c defined between the centres of the two rings.

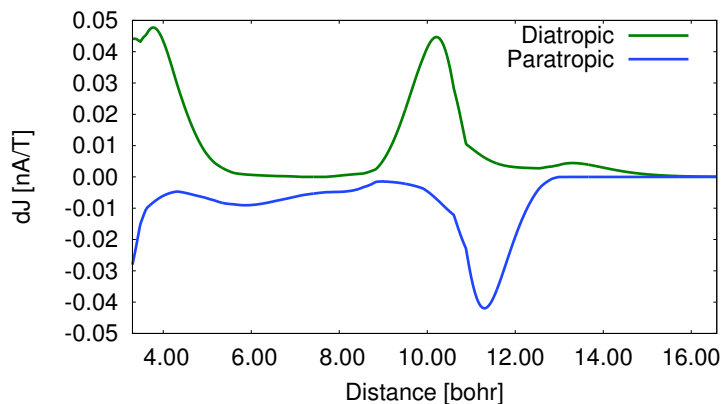
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-2.30	2.36	0.00
Diatropic domains		
-0.02	2.36	7.74
-0.04	0.96	2.8 / pm 0.3
Paratropic domains		
-2.30	0.00	-7.74



1.2 [10]annulene, twist conformation

Table 4 Plane a in the twist conformation of [10]annulene. The origin of the abscissa lies at the centre of the molecule and crosses a C – C bond.

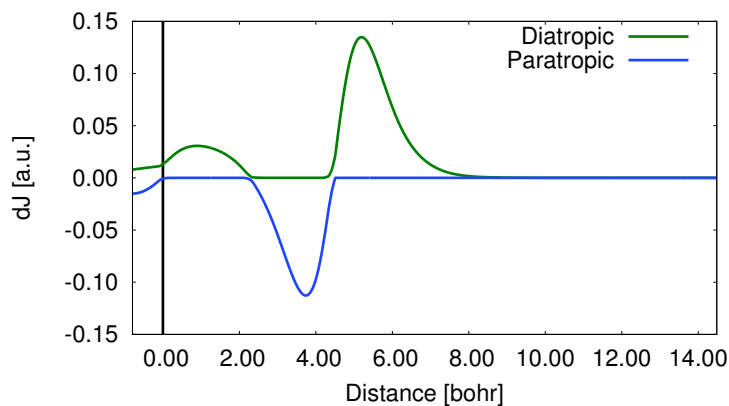
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
1.57	15.59	1.25
Diatropic domains		
1.57	15.59	11.87
Paratropic domains		
1.57	15.59	-10.62



1.3 [10]annulene, naphthalene-like conformation

Table 5 Plane a in the naphthalene-like conformation of [10]annulene. The origin of the plane lies at the centre of the molecule and crosses a C – C bond.

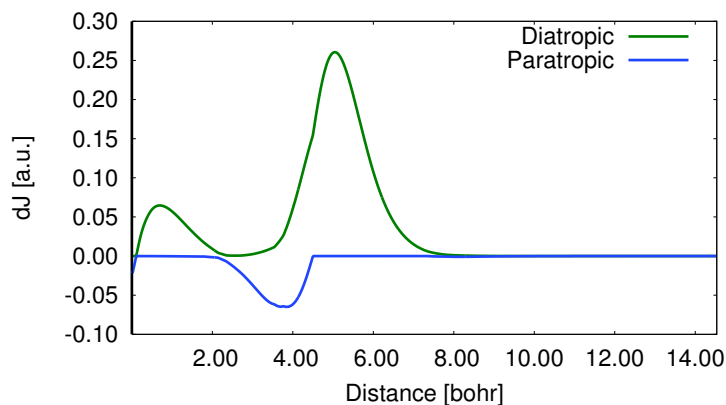
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
2.28	14.20	2.91
Diatropic domains		
2.28	14.20	-6.83
Paratropic domains		
2.28	14.20	-6.83



1.4 [10]annulene, heart-shaped conformation

Table 6 Plane a in the heart-shaped conformation of [10]annulene. The origin of the plane lies near the hydrogen atom pointing inwards to the ten-member ring and crosses a C – C bond.

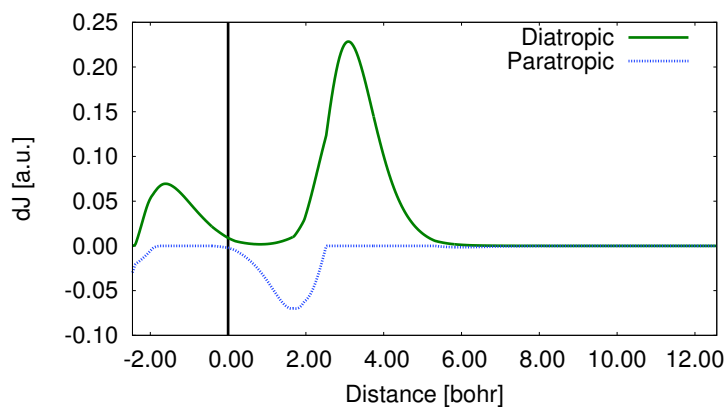
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
2.21	16.01	17.32
Diatropic domains		
0.01	2.55	3.95
2.21	16.01	21.87
Paratropic domains		
2.21	16.01	-4.55



1.5 [10]annulene, azulene-like conformation

Table 7 Plane a in the azulene-like conformation of [10]annulene. The origin of the integration plane lies between the two hydrogen atoms pointing in towards to ten-member ring.

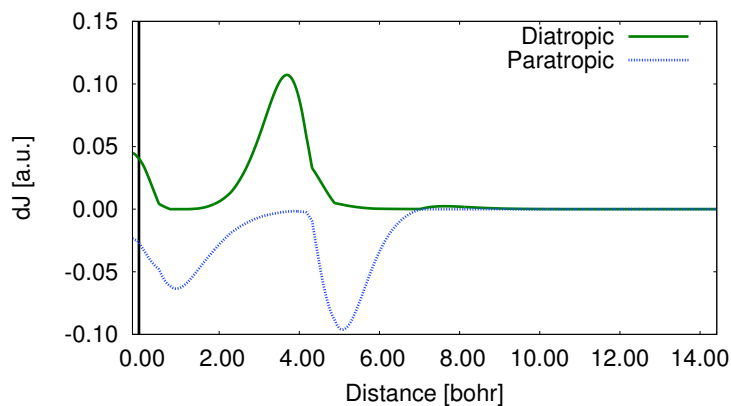
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.20	12.54	13.80
Diatropic domains		
0.82	12.54	18.60
Paratropic domains		
-0.40	12.54	-4.95



1.6 [10]annulene, boat conformation

Table 8 Plane a in the boat conformation of [10]annulene. The integration plane originates near the centre of the molecule.

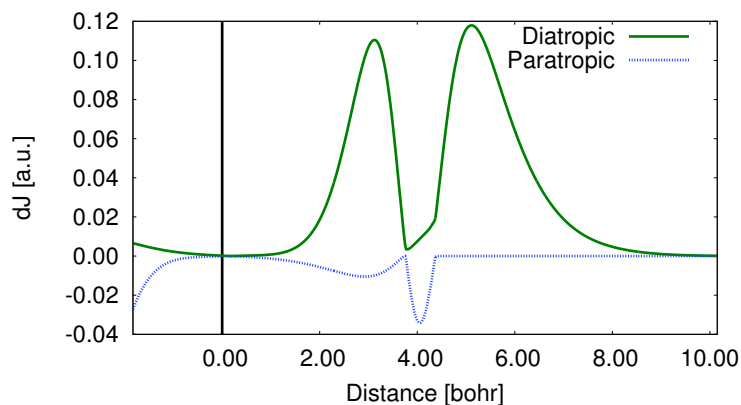
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
2.40	15.84	0.58
Diatropic domains		
0.80	6.84	7.57
Paratropic domains		
3.88	7.34	-6.39



1.7 [10]annulene, all-*trans* conformation

Table 9 The integration plane in the all-*trans* conformation of [10]annulene. The abscissa lies at the geometric centre of the molecule. The integration plane crosses a C – C bond.

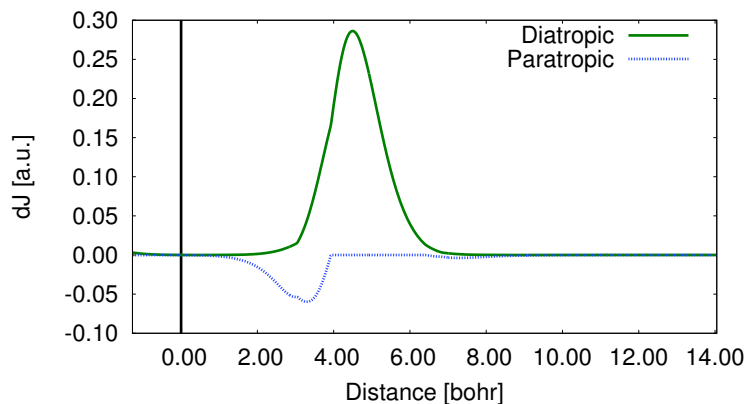
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.17	10.17	14.90
Diatropic domains		
0.17	10.17	16.41
0.17	3.79	6.24
3.79	10.17	10.18
Paratropic domains		
0.17	10.17	-1.52
3.75	4.39	-0.66



1.8 [10]annulene, all-*cis* conformation

Table 10 Plane **a** in the all-*cis* conformation of [10]annulene. The origin of the abscissa corresponds to the geometrical centre of the molecule.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.01	13.73	19.36
Diatropic domains		
0.47	13.73	23.90
Paratropic domains		
-0.07	3.95	-4.23



1.9 Molecule A_0

Table 11 Plane **a** with origin at the centre of the six-member ring and passing through atom C2.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.33	11.69	3.61
Diatropic domains		
0.33	11.69	12.14
1.57	11.69	11.95
2.47	3.95	3.91
Paratropic domains		
-0.01	11.69	-8.59
-0.01	2.47	-3.52

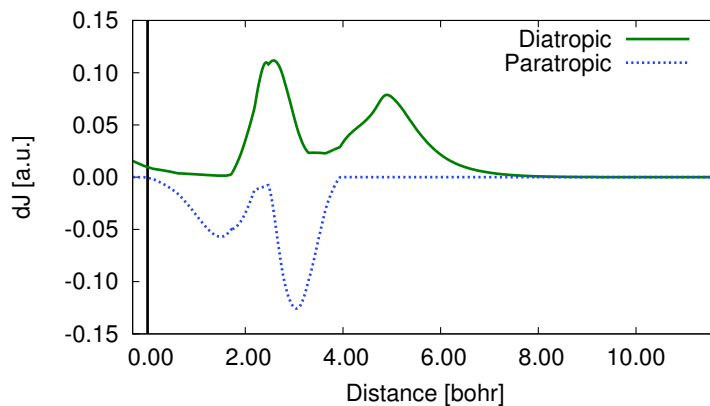


Table 12 Plane **b** with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.40	12.84	4.57
Diatropic domains		
-3.16	1.64	3.85
1.64	12.84	10.17
Paratropic domains		
0.10	2.58	-5.75

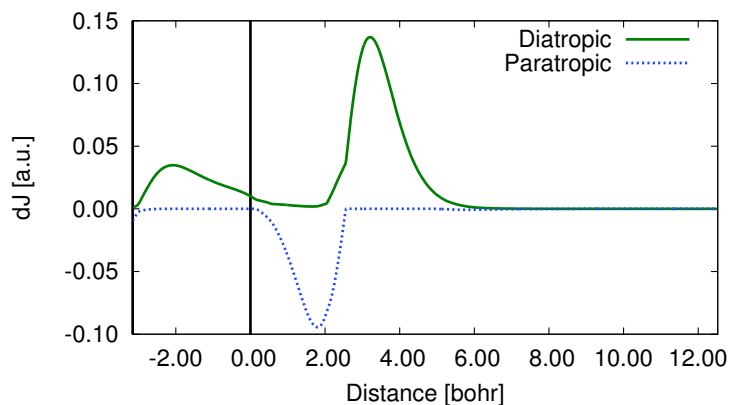


Table 13 Plane **c** with origin at the midpoint of the bond between the copper atoms and continuing along the bond to infinity. The range of the induced current strengths varies significantly, so a second plot with current strengths only in the range [-0.5:0.5] is provided.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.01	12.39	14.27
Diatropic domains		
0.01	12.39	217.84
1.19	2.33	156.70
3.01	12.39	2.01
Paratropic domains		
0.01	12.39	-203.57

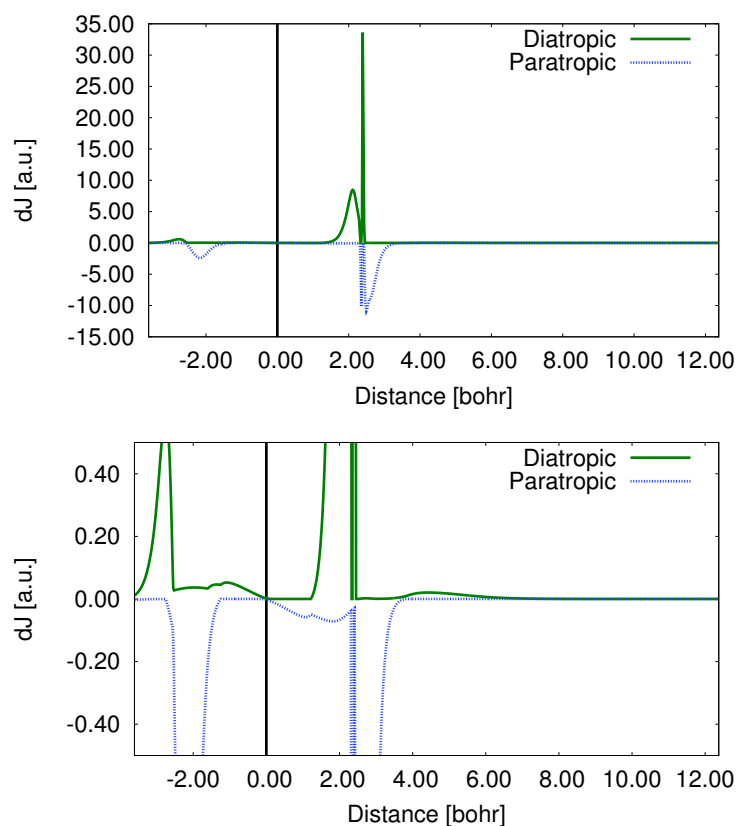
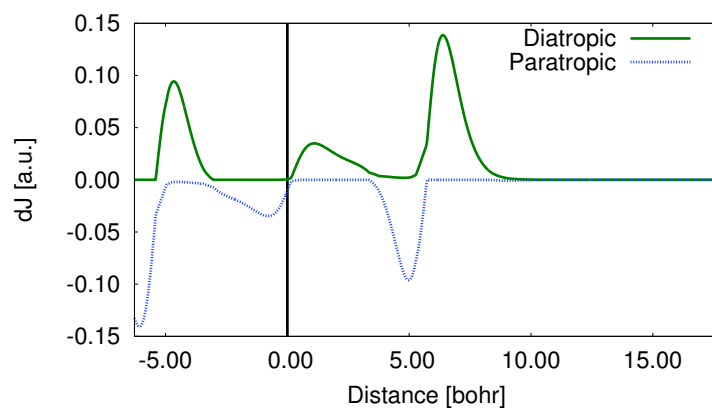


Table 14 Plane **d** defined between the centres of the two six-member rings.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-3.27	3.61	0.01
Diatropic domains		
-0.43	4.77	3.86
Paratropic domains		
-4.45	3.33	-3.86



1.10 Molecule A₂

Table 15 Plane **b** with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3. The vertical line at 2.72 bohr shows the geometrical centre of the six-member ring.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.03	15.63	-0.32
Diatropic domains		
-0.37	15.63	11.43
5.53	15.63	6.35
2.35*	5.53	3.1 ± 0.3
Paratropic domains		
0.03	15.63	-11.69
1.33	2.75	1.67
2.75	7.55	-8.03
-0.37	15.63	-11.43

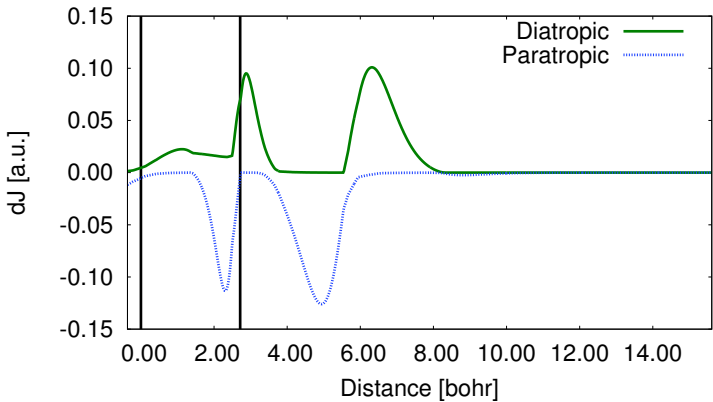
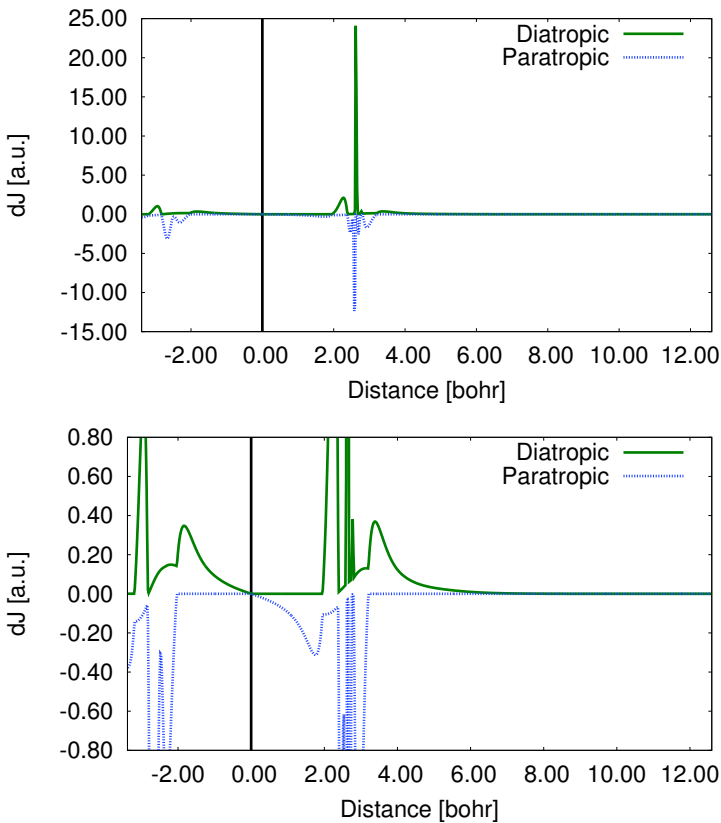


Table 16 Plane **c** passes between the two copper atoms. Its origin lies at the midpoint between the copper atoms. The range of the induced current strengths varies significantly, so a second plot with current strengths only in the range [-0.8:0.8] is provided.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.02	12.62	8.31
Diatropic domains		
0.02	12.62	86.40
Paratropic domains		
0.02	12.62	-78.09
0.00	1.94*	-11.8 ± 1.2
0.00	2.34*	-13.7 ± 1.4



1.11 Molecule A₄

Table 17 Plane **b** with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-3.10	12.90	15.13
-0.02	12.90	21.00
Diatropic domains		
-3.10	12.90	28.12
-3.10	-0.02	2.51
-0.02	12.90	25.61
Paratropic domains		
-3.10	12.90	-12.98
-1.42	0.12	-8.90
0.12	2.64	-3.99

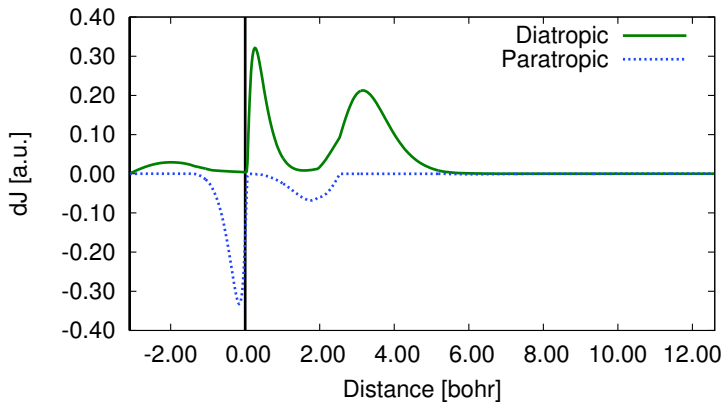
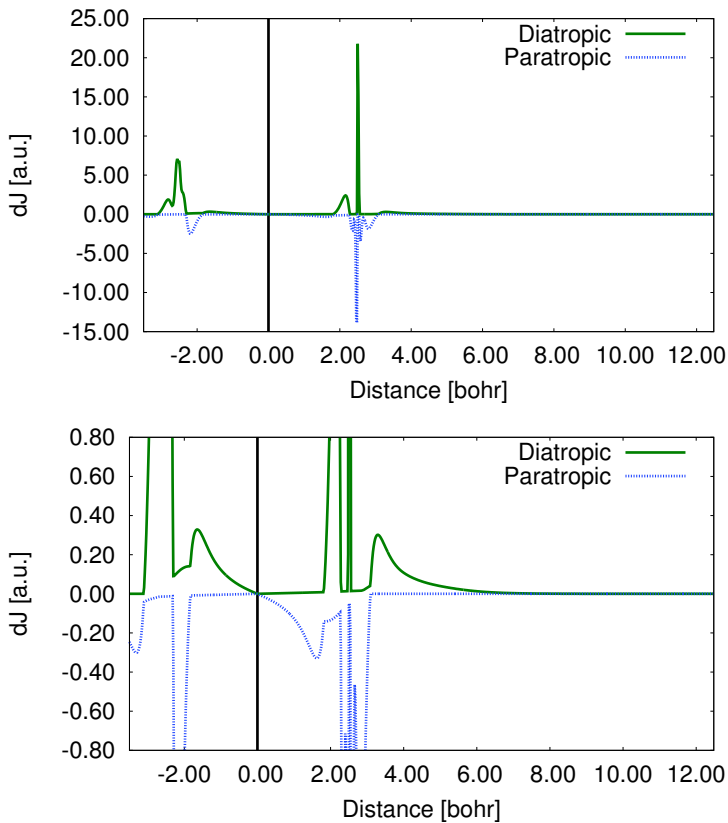


Table 18 Plane **c** passes through the two copper atoms. Its origin lies at the midpoint between the copper atoms and continuing to infinity. The range of the induced current strengths varies significantly, so a second plot with current strengths only in the range [-0.5:0.5] is provided.

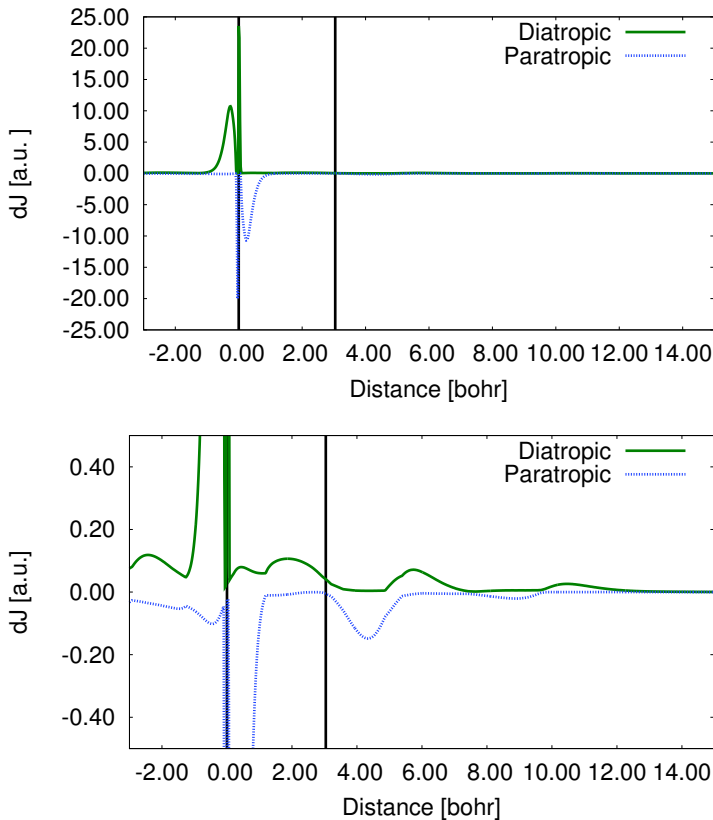
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
0.00	12.50	-6.31
Diatropic domains		
0.00	12.50	83.70
Paratropic domains		
0.00	12.50	-90.01



1.12 Molecule B₀

Table 19 Plane **b** with origin at the midpoint at the centre of Cu2. The second vertical line at $x = 3.04$ represents the centre of the five-member ring formed by the atoms Cu2, C5, C6, C7 and C8. The plane passes through the bond between atoms C6 and C7. The range of the induced current strengths varies significantly, so a second plot with current strengths only in the range [-0.4:0.4] is provided.

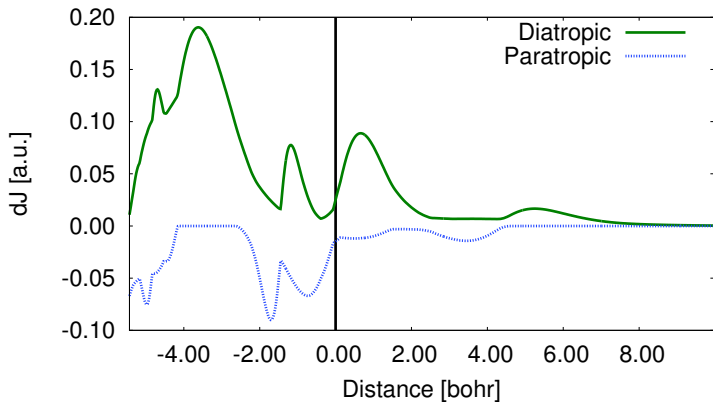
x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
3.30	15.00	-3.27
Diatropic domains		
3.30	15.00	8.28
4.40	10.57	5.7 ± 0.3
4.40	7.66	5.0 ± 0.3
Paratropic domains		
3.30	15.00	-11.55
3.30	5.18	-9.12



1.13 Molecule B₂

Table 20 Plane **a** with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-0.39	3.09	4.61
4.27	10.57	1.77
Diatropic domains		
-0.05	10.57	8.48
-0.39	3.09	6.46
4.27	10.57	1.80
Paratropic domains		
-0.39	3.09	-1.85
4.27	10.57	-0.03



1.14 Molecule B₄

Table 21 Plane **a** with origin at the centre of the six-member ring and passing through the midpoint between atoms C2 and C3. The profile on the first half of the plane, at $x < 0$, is reversed in sign. The diatropic contributions appear as paratropic and vice-versa. This is due to the viewpoint towards the direction of the current flow.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-14.26	-0.00	10.84
-0.00	25.74	10.67
7.64	25.74	1.77
Diatropic domains		
-14.26	-0.00	12.55
-0.00	25.74	25.85
-0.00	3.38	1.69
9.32	25.74	11.34
Paratropic domains		
-14.26	-0.00	-23.39
-0.00	25.74	-15.18
5.68	10.32	-10.13

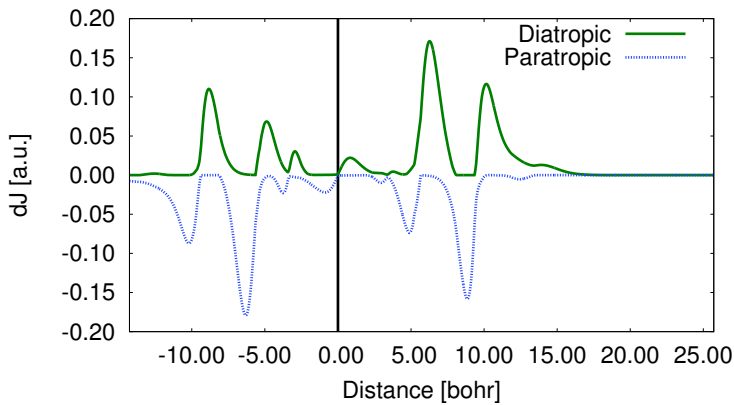
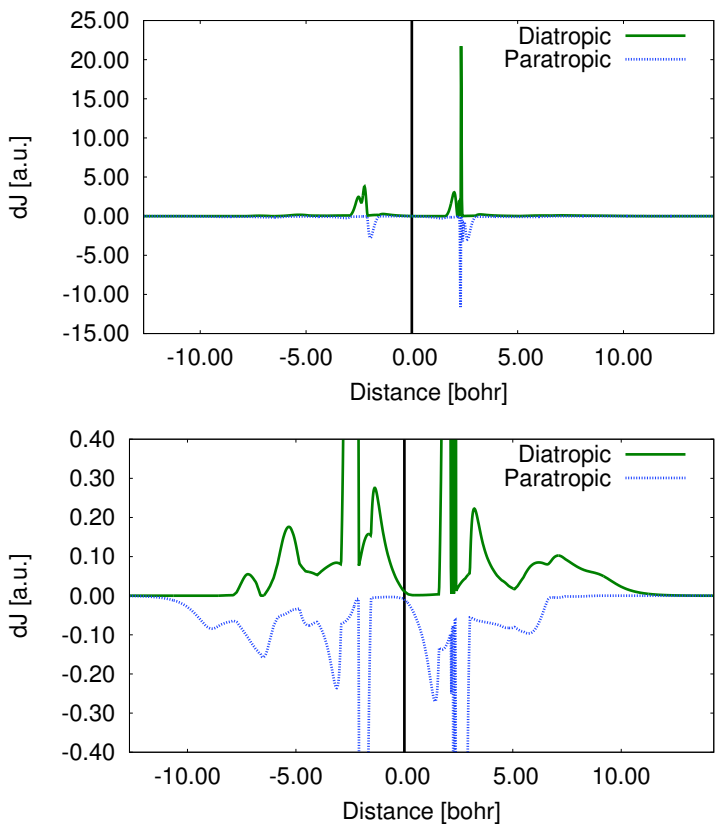


Table 22 Plane **b** with origin at the midpoint between the copper atoms.

x_1 [bohr]	x_2 [bohr]	current [nA/T]
Net current		
-12.67	0.03	30.27
0.03	14.33	9.26
Diatropic domains		
-12.67	0.03	103.62
0.03	14.33	111.56
Paratropic domains		
-12.67	0.03	-73.35
0.03	14.33	-102.30



2 Geometry of the optimized molecular structures.

2.1 Molecular coordinates

The molecular structures of the conformers of [10]annulenes were optimised at the SCS-MP2/def2-QZVPD level of theory. The geometries of the dicupra[10]annulenes were optimised at the BP86/def2-TZVP level of theory. The coordinates are listed in Å.

Twist conformation of [10]annulene

element	x	y	z
C	-0.9851407	-0.2821986	-1.1758527
C	-1.2502937	1.7714146	0.1395702
C	-0.0021675	2.2724783	0.0784053
C	1.2075539	1.5350744	-0.3150325
C	1.6198284	0.3427453	0.1384753
H	-1.9750896	-0.216196	0.6616508
H	-2.050628	2.4174569	0.4744943
H	0.1285748	3.3280051	0.2839526
H	1.8156535	2.0122832	-1.0740883
C	-1.5115391	0.3623894	-0.1274469
C	-0.6880786	-1.7090977	-1.1515727
C	-0.0516211	-2.2707161	-0.1065339
C	0.3529868	-1.5852247	1.1297436
C	1.0201088	-0.4275906	1.2398201
H	-0.5739193	0.2980502	-1.9922654
H	-0.9021804	-2.3224391	-2.016473
H	0.1380774	-3.3365647	-0.1446934
H	0.0534022	-2.0723806	2.0498598
H	2.4957842	-0.0909193	-0.3285715
H	1.1586881	-0.02657	2.2365585

Naphthalene-like conformation of [10]annulene

element	x	y	z
C	0.6606951	0.5826276	-2.2573955
C	0.7726212	1.4762849	-1.2472597
C	0.0529003	1.3345335	0.0031901
C	0.6582518	1.3764843	1.2015785
C	0.1876549	0.6479543	2.3812637
H	1.2308093	0.7880767	-3.1548498
H	1.5013569	2.2704647	-1.3454013
H	-0.9396669	0.9152294	-0.0623104
H	1.6588768	1.7924892	1.2626949
H	0.3608721	1.0925808	3.352817
C	-0.1559343	-0.6286207	-2.3024167
C	-0.4090519	-1.5018751	-1.2999783
C	0.1292207	-1.3339071	0.0355955
C	-0.6375845	-1.3525636	1.138321
C	-0.3352674	-0.5997229	2.3572141
H	-0.5954621	-0.8529311	-3.2663516
H	-1.1180788	-2.2989002	-1.4828494
H	1.121782	-0.9145685	0.1009052
H	-1.6375099	-1.7687118	1.0675221
H	-0.6430393	-1.0249243	3.3038347

Heart-shaped conformation of [10]annulene

element	x	y	z
C	-1.3357564	-1.3158988	0.0868671
H	0.1606236	0.1582198	-0.4878489
C	-2.0356576	-0.082851	0.0226028
C	-1.9471661	1.3205514	-0.0474477
C	-0.9719058	2.3194744	-0.0145316
C	0.4038427	2.1493106	0.0031774
H	-3.0893915	-0.3320436	0.0544952
H	-2.9428932	1.7443861	-0.0777597
H	-1.358093	3.3272596	0.05324
H	1.0569051	2.9886828	0.1978573
C	0.8928004	0.879523	-0.1790317
C	-0.1133286	-2.0341875	0.0225952
C	1.2912413	-1.9667249	-0.0474738
C	2.3046588	-1.0065365	-0.0145122
C	2.1551125	0.3716053	0.0032499
H	-0.3782727	-3.0840703	0.0545324
H	1.7001137	-2.968686	-0.0778914
H	3.3065472	-1.4077772	0.0532409
H	3.0041459	1.0120178	0.1980599
H	-2.1035233	-2.072254	0.1965801

Azulene-like conformation of [10]annulene.

element	x	y	z
C	-1.853772	1.2095539	0.0961165
C	-1.853747	-1.2095236	-0.0960441
C	0.5696903	-1.8960942	0.0377231
C	2.3217831	-0.000017	0.0000377
C	0.5696897	1.8960647	-0.0378015
H	-2.3394722	2.1418658	-0.1659264
H	-2.339361	-2.1417904	0.1663179
H	0.4212499	-2.8667658	0.494541
H	3.4061676	0.0000142	0.0002838
H	0.4212544	2.8666972	-0.4947039
C	-2.5567752	0.0000069	-0.0000477
C	-0.5013572	-1.1708239	-0.4467123
C	1.8421401	-1.321401	0.1349508
C	1.8421261	1.3213549	-0.1350032
C	-0.5013748	1.1708528	0.4467074
H	-3.638255	0.0000101	-0.0002767
H	-0.2140111	-0.3017688	-1.0171271
H	2.6270202	-2.0117197	0.4209783
H	2.6269868	2.0116257	-0.4211991
H	-0.2140278	0.3018673	1.0172235

Boat conformation of [10]annulene

element	x	y	z
C	-1.8539962	0.4197465	0.7312381
C	0.1475589	-0.8312758	1.8073504
C	1.5469301	0.8718536	0.6669503
C	-1.116478	-0.0988696	-1.7304306
C	1.3405189	-0.3760573	-1.4215244
H	-2.7358707	0.9289007	1.0991224
H	0.1153471	-1.7588808	2.3659027
H	1.7289769	1.7909159	1.2081665
H	-1.55908	0.047992	-2.7102594
H	2.2139942	-0.9764538	-1.644261
C	-1.1166323	-0.0994486	1.7303078
C	1.340645	-0.3756399	1.4216549
C	-1.853813	0.4202363	-0.7313124
C	0.1473309	-0.8314084	-1.807224
C	1.5469357	0.8716465	-0.6671856
H	-1.5596859	0.0466551	2.710046
H	2.2142525	-0.9757248	1.644725
H	-2.7353314	0.9300613	-1.0991191
H	0.1147734	-1.7591855	-2.3654677
H	1.7289259	1.7905564	-1.2086799

All-cis conformation of [10]annulene

element	x	y	z
C	2.2563237	-0.0000003	0.0000098
H	3.3392755	0.0000008	-0.0000054
C	1.8254091	1.3262372	-0.000005
C	0.697243	2.145892	-0.0000004
C	-0.6972433	2.1458919	0.0000121
C	-1.8254087	1.3262371	-0.0000151
C	-2.2563224	0.0000001	0.00001
C	-1.8254094	-1.326238	-0.0000049
C	-0.697243	-2.1458917	-0.0000005
C	0.6972425	-2.1458912	0.0000121
C	1.8254091	-1.3262382	-0.0000153
H	2.7015343	1.9627725	0.000002
H	1.0318942	3.1758372	0.000004
H	-1.031895	3.1758361	-0.0000028
H	-2.7015348	1.9627719	0.0000006
H	-3.3392736	0.0000007	-0.0000049
H	-2.7015357	-1.9627722	0.0000012
H	-1.0318944	-3.1758368	0.0000042
H	1.0318936	-3.1758356	-0.0000026
H	2.7015354	-1.9627733	0.0000008

All-trans conformation of [10]annulene

element	x	y	z
H	1.86541	-0.6063047	1.4098634
C	1.9126043	-0.6216831	0.3273498
C	1.9127669	0.6212596	-0.3274796
H	1.8655439	0.6059298	-1.4099894
H	1.1530762	1.5866528	1.4098989
C	1.1823091	1.6268357	0.3273864
C	0.0002445	2.0110818	-0.3274136
H	0.0002013	1.9615249	-1.4099356
H	-1.1526349	1.5869777	1.4099756
C	-1.1818636	1.6271476	0.3274614
C	-1.9125866	0.6216964	-0.3273316
H	-1.8653466	0.6063017	-1.4098424
H	-1.8655929	-0.6059948	1.4099813
C	-1.9127794	-0.6212509	0.3274684
C	-1.1822719	-1.6268401	-0.3273996
H	-1.1531374	-1.5866178	-1.4099052
H	-0.0002328	-1.9615385	1.4099204
C	-0.0002532	-2.0110851	0.3273988
C	1.1818948	-1.6271298	-0.3274448
H	1.1526484	-1.5869631	-1.4099626

Molecule A₀

element	x	y	z
C	-7.467905078	0.917777452	0.21187075
C	-7.467626328	2.266702407	-0.056151325
C	-6.313808132	3.119191707	-0.09421111
H	-8.431817759	2.780563666	-0.184530016
C	-5.014544547	2.732230381	0.135142781
H	-6.527918713	4.186976423	-0.248931662
C	-2.804769359	-0.266395155	-0.226627849
C	-5.267931919	-2.069278521	-0.254264518
C	-3.976636627	-2.467293445	0.000860091
Cu	-4.11456581	1.081913317	-0.04521458
H	-4.34007181	3.576944122	0.369206017
Cu	-6.154291054	-0.418442383	-0.021941953
H	-8.460398365	0.525934562	0.501353087
H	-5.939975303	-2.902257276	-0.531397473
C	-2.819026756	-1.619446086	0.017238869
H	-1.80028611	0.124286441	-0.474232171
H	-3.771437348	-3.539512228	0.136330323
H	-1.861837095	-2.140256861	0.166594932

Molecule A₂

element	x	y	z
C	-7.550728985	0.929446941	0.200693682
C	-7.486044861	2.25704595	-0.122203494
C	-6.290806489	3.137344794	-0.13464845
H	-8.412879509	2.796187457	-0.36200043
C	-4.999566212	2.808626923	0.174535423
H	-6.533994279	4.179904594	-0.381876354
C	-2.724762456	-0.278438181	0.11040419
C	-5.276043623	-2.15755089	0.132197022
C	-3.995725879	-2.479955631	-0.22531395
Cu	-4.0205461	1.145423208	0.284746135
H	-4.333700968	3.686705764	0.1535219
Cu	-6.250369438	-0.497027367	0.305716223
H	-8.58690639	0.553762651	0.197652625
H	-5.942517932	-3.035276446	0.116311625
C	-2.800439082	-1.599691401	-0.235335176
H	-1.689110124	0.097515148	0.080552316
H	-3.76111206	-3.517555656	-0.500153964
H	-1.882143606	-2.133924209	-0.515580647
Li	-4.043176351	-1.143825085	1.515926846
Li	-6.186853977	1.768440112	1.578541985

Molecule A₄

element	x	y	z
C	-7.506961763	0.929838073	0.011569807
C	-7.525941537	2.336531833	0.025235988
C	-6.352986135	3.20139444	0.013550328
H	-8.485332829	2.867784853	0.046301614
C	-5.015492609	2.766252336	-0.013283806
H	-6.576177007	4.275105438	0.027445744
C	-2.774407265	-0.275407489	-0.076737332
C	-5.266232524	-2.111630104	-0.054247324
C	-3.928573872	-2.546230599	-0.080668049
Cu	-4.076098512	1.111776587	-0.043793727
H	-4.311812775	3.613251146	-0.016946016
Cu	-6.206571814	-0.45851334	-0.022297026
H	-8.525138801	0.510462709	0.024465619
H	-5.968853917	-2.959691716	-0.05210507
C	-2.755369648	-1.681995645	-0.090910153
H	-1.756679601	0.144916169	-0.088852905
H	-3.705968256	-3.620304794	-0.095584544
H	-1.796249249	-2.213901372	-0.112048957
Li	-4.124667011	-1.032636454	1.457855236
Li	-4.171975203	-1.005471033	-1.582044817
Li	-6.107913197	1.660156605	1.514738079
Li	-6.157316137	1.686422898	-1.523362745

Molecule B₀

element	x	y	z
C	-1.171168088	2.38885318	-0.250057019
C	-2.101580158	1.59220012	0.374119028
C	-2.318005175	0.232547018	-0.156980012
C	-1.59049912	-0.195339015	-1.262011095
Cu	0.077868006	-1.186147089	-1.310123099
Cu	-0.072611006	1.18841409	-1.305311098
C	1.59560912	0.197459015	-1.260285095
C	1.172800088	-2.38797118	-0.252478019
C	2.100074158	-1.59145312	0.376395028
C	2.319932175	-0.231942018	-0.153889012
Si	-2.345424177	-0.92315507	-2.834337214
Si	-0.66186805	4.146332313	0.154131012
Si	2.351838177	0.92807007	-2.830425213
Si	0.66430205	-4.146909313	0.146524011
C	-0.780675059	-4.579098345	-0.991127075
H	-1.567049118	-3.813075287	-0.948411072
H	-1.227905093	-5.548942418	-0.726865055
H	-0.435532033	-4.64028735	-2.034207153
C	0.117727009	-4.265166322	1.953098147
H	-0.689223052	-3.553558268	2.179154164
H	0.962034073	-4.037048304	2.619437197
H	-0.244374018	-5.278614398	2.184493165
C	2.014679152	-5.43255041	-0.179847014
H	2.544122192	-5.225626394	-1.121211085
H	1.561779118	-6.432742485	-0.26033602
H	2.751321207	-5.456125411	0.633771048
C	-3.768918284	-2.112452159	-2.52449819
H	-3.425974258	-3.016595227	-2.004189151
H	-4.209945317	-2.413408182	-3.487494263
H	-4.554304343	-1.651362125	-1.910615144
C	-1.047465079	-1.782696134	-3.909318295
H	-0.684057052	-2.721957205	-3.468037261
H	-0.180305014	-1.137667086	-4.11158031
H	-1.502464113	-2.030021153	-4.881792368
C	-0.113539009	4.255715321	1.960766148
H	-0.957952072	4.025215303	2.626203198
H	0.249490019	5.267769397	2.196780166
H	0.692836052	3.542358267	2.183398165
C	-2.010651152	5.43558341	-0.164230012
H	-2.747203207	5.454905411	0.649591049
H	-2.540497192	5.235334395	-1.106841083
H	-1.556467117	6.435699485	-0.238446018
C	0.782327059	4.581035345	-0.983569074
H	1.567444118	3.813436287	-0.944670071
H	1.231606093	5.549101418	-0.716290054
H	0.435947033	4.64664635	-2.025965153
C	1.05479108	1.791848135	-3.903001294
H	0.693764052	2.731065206	-3.459683261
H	0.185983014	1.148805087	-4.104965309
H	1.508907114	2.039675154	-4.875745368
C	2.968590224	-0.592778045	-3.762327284
H	3.357998253	-0.326480025	-4.756532359
H	2.157766163	-1.3246381	-3.887285293
H	3.769641284	-1.082517082	-3.190138241
C	3.776851285	2.114776159	-2.51745219
H	3.435102259	3.018316228	-1.99532315
H	4.218693318	2.417166182	-3.479621262
H	4.561257344	1.651109125	-1.904299144
C	2.851136215	-2.037355154	1.58553312
C	3.32245225	0.680767051	0.440900033
C	-2.860106216	2.038223154	1.578529119
C	-3.31880025	-0.683080052	0.436227033
C	4.658956351	0.303435023	0.66481305
C	3.813251287	-3.05579823	1.512601114
C	-4.656950351	-0.310244023	0.65815605

element	x	y	z
C	2.924893221	1.98769615	0.771732058
C	2.584452195	-1.45230511	2.834700214
C	-2.91729822	-1.98854315	0.768066058
C	-5.56943242	-1.235185093	1.164182088
H	-4.982164376	0.700633053	0.414223031
C	5.57386542	1.225320092	1.172010088
H	4.981047376	-0.708545053	0.421412032
C	4.472324337	-3.500101264	2.660884201
H	4.045501305	-3.491862263	0.540530041
C	3.835684289	2.903775219	1.293641098
H	1.880966142	2.25805717	0.614087046
C	5.16741239	2.526756191	1.487907112
H	6.612183498	0.92663307	1.3230241
C	3.238665244	-1.896853143	3.9833693
H	1.85024414	-0.647403049	2.896366218
C	4.182814315	-2.925831221	3.901458294
H	5.217220393	-4.293999324	2.585596195
C	-5.159025389	-2.535228191	1.480781112
H	-6.608979498	-0.940011071	1.313675099
C	-3.825727288	-2.907749219	1.288590097
H	-1.872053141	-2.25519317	0.612458046
H	-3.489669263	-3.914119295	1.542495116
H	-5.876509443	-3.251749245	1.882912142
H	3.011083227	-1.439813109	4.947653373
H	4.694322354	-3.273425247	4.799978362
H	3.502682264	3.911296295	1.547028117
H	5.886723444	3.240840244	1.891102143
C	-3.823597288	3.05483023	1.498483113
C	-2.600706196	1.45447411	2.829874213
C	-4.491671339	3.498187264	2.641929199
H	-4.049744305	3.490151263	0.52464104
C	-3.263936246	1.898106143	3.9737393
H	-1.865416141	0.651003049	2.897039218
C	-4.209800317	2.924924221	3.884723293
H	-5.237652395	4.290537323	2.561064193
H	-3.042206229	1.441894109	4.939783372
H	-4.728585356	3.271593247	4.77943036
C	-2.963695223	0.599443045	-3.762280284
H	-2.153542162	1.3324041	-3.884990293
H	-3.765344284	1.086810082	-3.18883024
H	-3.352692253	0.335489025	-4.757281359

Molecule B₂

element	x	y	z
C	-5.794578593	4.775684223	1.500166218
C	-6.968502265	4.358643712	0.909259251
C	-7.017741104	3.257820491	-0.129339963
C	-6.039023535	2.298804389	-0.311137927
Cu	-4.320595774	1.886115326	0.511500483
Cu	-4.159363923	4.236339357	0.626875012
C	-2.504973467	3.914548059	-0.352852379
C	-2.630681324	1.266217705	1.209952836
C	-1.499312069	1.744983856	0.583784052
C	-1.519355913	2.945598626	-0.338899615
Si	-5.909436177	1.182450171	-1.829231516
Si	-5.584689106	5.924454865	2.95509523
Si	-2.737574918	5.178907037	-1.736805722
Si	-2.743738712	-0.023318416	2.552999179
C	-4.236254232	0.498495725	3.613796018
H	-4.135884295	1.542367276	3.952205597
H	-4.368286536	-0.136731373	4.502236435
H	-5.147785251	0.415891533	2.997620871
C	-1.252364267	-0.152924381	3.710283695
H	-1.006596264	0.826914122	4.147632267
H	-0.358656591	-0.511993793	3.18229404
H	-1.466024403	-0.844020642	4.540131429
C	-3.155774365	-1.711766899	1.814274744
H	-3.948199525	-1.605073782	1.058410345
H	-3.509603543	-2.409298093	2.588337377
H	-2.278120718	-2.160156247	1.328375421
C	-6.565692186	-0.539447372	-1.410894268
H	-6.102402482	-0.899614168	-0.479958399
H	-6.329710628	-1.257507492	-2.210686804
H	-7.656015375	-0.529660219	-1.271761247
C	-4.060213463	1.010868195	-2.244855483
H	-3.512656267	0.379088099	-1.529253512
H	-3.559616396	1.989791129	-2.269653996
H	-3.958312576	0.554447829	-3.242304621
C	-6.99063866	5.928551864	4.221432626
H	-7.918550508	6.334699244	3.796589934
H	-6.717764939	6.533104831	5.100045267
H	-7.207079368	4.908180048	4.573360459
C	-5.223643471	7.681373297	2.363954735
H	-6.132933659	8.171487252	1.989237768
H	-4.486629436	7.656936866	1.547354637
H	-4.815309809	8.298794797	3.178216282
C	-4.021841151	5.307351468	3.850406918
H	-4.100193005	4.234547065	4.089725975
H	-3.825851991	5.851834292	4.786039664
H	-3.155976393	5.455127633	3.182635095
C	-4.610830768	5.380527631	-2.004472068
H	-5.10626397	5.935082184	-1.193111034
H	-5.113219367	4.406075706	-2.091129184
H	-4.781666121	5.933006875	-2.942098432
C	-2.050224699	4.703542138	-3.432460011
H	-2.430608558	5.412728262	-4.184263563
H	-2.388754711	3.697165371	-3.718977195
H	-0.953835321	4.709647432	-3.473273472
C	-2.052448949	6.852709046	-1.189565234
H	-2.451930106	7.113048175	-0.197732579
H	-2.340693822	7.647435185	-1.894052398
H	-0.955235951	6.83497701	-1.125298847
C	-0.177708302	1.068299281	0.769270508
C	-0.375350337	3.008813746	-1.297914696
C	-8.271476501	5.008530864	1.254163948
C	-8.226487643	3.28813571	-1.007060082
C	-0.216364729	2.013929098	-2.274701885
C	-0.029435292	-0.280177115	0.410362877
C	-8.44994703	4.376338952	-1.864428596

element	x	y	z
C	0.542058172	4.068927854	-1.261941409
C	0.921817862	1.732160366	1.334841852
C	-9.142824881	2.226532211	-1.014609621
C	-9.539533833	4.38349298	-2.73465558
H	-7.742825039	5.207393891	-1.858005473
C	0.809736472	2.098742603	-3.215165249
H	-0.92424887	1.184016552	-2.303094592
C	1.1688234	-0.956819931	0.641050227
H	-0.871620771	-0.790857764	-0.058248402
C	1.580246419	4.148804808	-2.191898564
H	0.428371974	4.838244913	-0.496128806
C	1.711959338	3.166982741	-3.177667482
H	0.906883115	1.32935636	-3.982713472
C	2.116119023	1.055969227	1.584842366
H	0.839784034	2.793261095	1.582088164
C	2.242805806	-0.293653125	1.241551951
H	1.264759893	-2.004930112	0.353308692
C	-10.44046423	3.313536537	-2.742827868
H	-9.687434777	5.22634096	-3.411614984
C	-10.24363613	2.237435411	-1.873162112
H	-8.978695778	1.384113219	-0.340377995
H	-10.94589308	1.402305311	-1.867702099
H	-11.29458599	3.32127682	-3.421209142
H	2.953326327	1.583670599	2.044258507
H	3.178084918	-0.821760256	1.431229136
H	2.284311498	4.981424006	-2.150849567
H	2.516661639	3.230864173	-3.911266086
Li	-2.253977219	3.4109291	1.729265361
Li	-6.140450248	2.587228335	1.823778516
C	-8.440300677	6.385520759	1.042973491
C	-9.330572883	4.287350714	1.826716135
C	-9.617107498	7.031181313	1.42398815
H	-7.631673176	6.943681573	0.569413709
C	-10.5020651	4.930651763	2.226502084
H	-9.234650836	3.207218496	1.960665219
C	-10.64823605	6.307307431	2.029426589
H	-9.729685541	8.102415338	1.249840562
H	-11.30651848	4.356581497	2.688820698
H	-11.56606454	6.810289424	2.33635885
C	-6.709022766	1.828281199	-3.415767425
H	-6.384962353	2.85898731	-3.620856642
H	-7.805626875	1.825229404	-3.380873544
H	-6.385782186	1.199945415	-4.260442309

Molecule B₄

element	x	y	z
C	-5.785444737	4.879996966	0.680181467
C	-7.092617156	4.33492309	0.516343185
C	-7.37800359	2.982406718	-0.027580144
C	-6.386077198	1.994311545	-0.296832786
Cu	-4.492836147	1.876225768	0.057027661
Cu	-4.023285608	4.290329031	0.160258062
C	-2.159785164	4.217249503	-0.334833555
C	-2.699664626	1.243654395	0.383233022
C	-1.405802609	1.80757954	0.181523954
C	-1.154924681	3.210343358	-0.239281816
Si	-6.76180798	0.47201753	-1.354527374
Si	-5.475010577	6.414615901	1.741247391
Si	-1.853297526	5.842237375	-1.252788957
Si	-2.937536051	-0.394221125	1.298600448
C	-4.469600301	-0.26155072	2.422428267
H	-4.309571853	0.525625187	3.176670818
H	-4.638588435	-1.211631186	2.95472996
H	-5.38041667	-0.009854264	1.861114864
C	-1.562064099	-0.880841103	2.511134598
H	-1.271335671	-0.03749999	3.155020953
H	-0.65389607	-1.246012049	2.015258414
H	-1.944511661	-1.681917605	3.163542133
C	-3.215497961	-1.859477758	0.135497208
H	-4.058818872	-1.689178625	-0.546175337
H	-3.432093957	-2.767267311	0.719334008
H	-2.319334501	-2.055822064	-0.469902995
C	-7.073179841	-1.085053677	-0.327123455
H	-6.239436434	-1.301707525	0.353201461
H	-7.20137957	-1.95417488	-0.990494327
H	-7.988196304	-0.983192513	0.273268525
C	-5.271458451	0.117738669	-2.486468209
H	-4.343154847	-0.040121162	-1.919611005
H	-5.111196064	0.96971847	-3.166659009
H	-5.461140716	-0.77635217	-3.102275386
C	-6.756413738	6.766780668	3.095211098
H	-7.697315204	7.177608156	2.707991022
H	-6.324251395	7.497307392	3.797520101
H	-7.001829298	5.859898804	3.667739419
C	-5.276764701	7.994211986	0.720161401
H	-6.213471596	8.249159112	0.204606957
H	-4.48547881	7.899088274	-0.034694586
H	-5.015132216	8.836977287	1.378338551
C	-3.865688986	6.171792047	2.73056298
H	-3.973643397	5.310544266	3.409417774
H	-3.654375129	7.062488639	3.344260251
H	-2.999402182	5.982481642	2.081151483
C	-3.418512006	6.308949003	-2.23254682
H	-4.303790728	6.402877103	-1.587922438
H	-3.630108172	5.533444406	-2.98616759
H	-3.26901434	7.263956895	-2.761929231
C	-0.510040921	5.80380429	-2.591841291
H	-0.624642633	6.700429443	-3.221544319
H	-0.61223863	4.923781102	-3.244197597
H	0.509290952	5.797293957	-2.185705645
C	-1.462295444	7.285483257	-0.09464428
H	-2.246059062	7.430508187	0.660132375
H	-1.374526371	8.218291603	-0.672641943
H	-0.508862542	7.12342025	0.427667721
C	-0.194459372	0.941358024	0.345088951
C	0.271567792	3.568236138	-0.524973799
C	-8.285913174	5.174327712	0.85722875
C	-8.822481598	2.6506266	-0.246998619
C	0.991717925	2.990737701	-1.582090434
C	-0.020014499	-0.171750703	-0.492292946
C	-9.6135777	3.33213948	-1.184770413

element	x	y	z
C	0.920215967	4.522907382	0.274108582
C	0.779550263	1.19235263	1.32382207
C	-9.416506411	1.615862767	0.492662453
C	-10.94540619	2.977359865	-1.394593697
H	-9.177676576	4.155368975	-1.753501239
C	2.306697131	3.370156958	-1.847550915
H	0.513632915	2.229493304	-2.200955835
C	1.080661857	-1.017301927	-0.348759319
H	-0.766834906	-0.371979891	-1.262795672
C	2.238459498	4.902390647	0.018536116
H	0.37283859	4.972601332	1.104594564
C	2.935927791	4.33035985	-1.049268184
H	2.844007444	2.915967155	-2.681367756
C	1.878064903	0.347816481	1.477546864
H	0.674876267	2.065756084	1.96977586
C	2.032594985	-0.763257661	0.642798099
H	1.195345015	-1.876917833	-1.010933408
C	-11.52007228	1.937203894	-0.657699797
H	-11.53865486	3.513562419	-2.136757095
C	-10.75091578	1.260158279	0.293048566
H	-8.813307098	1.08434727	1.231050431
H	-11.19129147	0.45218607	0.879421884
H	-12.56208568	1.659328062	-0.82070326
H	2.617391332	0.555840822	2.252371226
H	2.891984831	-1.424186797	0.761909717
H	2.722166299	5.646834059	0.652886813
H	3.964835998	4.627427163	-1.255826338
Li	-2.397469177	3.128658568	1.527560008
Li	-2.682519897	2.376964911	-1.469381953
Li	-6.012746345	2.887447483	1.646295253
Li	-5.943631928	3.946380989	-1.273245553
C	-8.517561593	6.368209744	0.155991511
C	-9.186898021	4.817865644	1.872546516
C	-9.602354781	7.188966895	0.466907827
H	-7.828183201	6.651594947	-0.641576349
C	-10.26878631	5.636554577	2.193346426
H	-9.038359725	3.882019758	2.414116238
C	-10.48037524	6.828128467	1.492947892
H	-9.762327729	8.112599706	-0.091572678
H	-10.95049756	5.345050425	2.993696259
H	-11.32694082	7.468875312	1.742642623
C	-8.196965932	0.642131338	-2.583646098
H	-8.138580147	1.58463742	-3.148194915
H	-9.184891093	0.602885496	-2.107758457
H	-8.130302535	-0.184863503	-3.308413316

3 Nuclear shielding constants

3.1 [10]annulene in different conformations

Twist		Naphthalene-like		Heart-shaped		Azulune-like	
Index	Shielding constant	Index	Shielding constant	Index	Shielding constant	Index	Shielding constant
1 c	53.78	1 c	51.14	1 c	42.48	1 c	37.90
2 h	36.65	2 c	45.12	2 c	43.52	2 c	37.90
3 c	52.91	3 c	17.73	3 c	44.06	3 c	52.16
4 c	54.19	4 c	44.30	4 c	48.54	4 c	56.69
5 c	48.91	5 c	44.84	5 c	42.19	5 c	52.15
6 c	49.56	6 h	25.02	6 h	25.69	6 h	23.38
7 h	23.24	7 h	24.55	7 h	25.59	7 h	23.38
8 h	23.59	8 h	28.14	8 h	25.53	8 h	24.22
9 h	23.62	9 h	24.89	9 h	25.73	9 h	24.45
10 h	23.13	10 h	25.10	10 c	42.47	10 h	24.21
11 c	40.77	11 c	51.13	11 c	43.52	11 c	40.53
12 c	52.91	12 c	45.14	12 c	44.06	12 c	13.74
13 c	54.19	13 c	17.76	13 c	48.54	13 c	47.03
14 c	48.92	14 c	44.31	14 c	42.20	14 c	47.01
15 c	49.55	15 c	44.85	15 h	25.69	15 c	13.75
16 h	23.24	16 h	25.02	16 h	25.59	16 h	23.84
17 h	23.59	17 h	24.55	17 h	25.53	17 h	33.46
18 h	23.62	18 h	28.14	18 h	25.73	18 h	24.42
19 h	23.13	19 h	24.89	19 h	25.74	19 h	24.41
20 h	23.28	20 h	25.10	20 h	25.74	20 h	33.46

Boat		All- <i>cis</i>		All- <i>trans</i>	
Index	Shielding constant	Index	Shielding constant	Index	Shielding constant
1 c	52.18	1 c	-43.85	1 h	27.63
2 c	44.13	2 h	26.75	2 c	18.54
3 c	44.50			3 c	18.54
4 c	46.33			4 h	27.63
5 c	46.88			5 h	27.63
6 h	26.26			6 c	18.54
7 h	25.62			7 c	18.55
8 h	25.15			8 h	27.63
9 h	26.20			9 h	27.63
10 h	26.30			10 c	18.54
11 c	46.33			11 c	18.54
12 c	46.88			12 h	27.63
13 c	52.17			13 h	27.63
14 c	44.13			14 c	18.54
15 c	44.50			15 c	18.54
16 h	26.20			16 h	27.63
17 h	26.30			17 h	27.63
18 h	26.26			18 c	18.55
19 h	25.62			19 c	18.54
20 h	25.15			20 h	27.63

3.2 Dicupra[10]annulenes

Table 23 Nuclear shielding constants for the unsubstituted dicupra[10]annulenes.

Molecule (A_0)	Shielding constant	Molecule (A_2)	Shielding constant	Molecule (A_4)	Shielding constant
Index		Index		Index	
1 c	67.88	1 c	23.62	1 c	68.67
2 c	7.92	2 c	27.54	2 c	70.65
3 c	47.72	3 c	27.56	3 c	70.61
4 h	23.44	4 h	23.96	4 h	23.23
5 c	35.04	5 c	23.59	5 c	68.67
6 h	24.88	6 h	23.96	6 h	23.23
7 c	67.99	7 c	23.55	7 c	68.65
8 c	34.93	8 c	23.52	8 c	68.62
9 c	47.63	9 c	27.67	9 c	70.65
10 cu	-841.47	10 cu	704.13	10 cu	268.65
11 h	24.77	11 h	25.19	11 h	23.673
12 cu	-844.24	12 cu	704.04	12 cu	267.4
13 h	26.51	13 h	25.19	13 h	23.68
14 h	24.76	14 h	25.19	14 h	23.68
15 c	7.80	15 c	27.66	15 c	70.63
16 h	26.51	16 h	25.19	16 h	23.67
17 h	24.88	17 h	23.95	17 h	23.23
18 h	23.43	18 h	23.95	18 h	23.23
		19 li	85.62	19 li	99.53
		20 li	85.62	20 li	99.53
				21 li	99.53
				22 li	99.53

Table 24 Nuclear shielding constants for the substituted dicupra[10]annulenes.

Molecule (B_0)	Shielding constant	Molecule (B_2)	Shielding constant	Molecule (B_4)	Shielding constant
Index		Index		Index	
1 c	-73.54	1 c	-27.32	1 c	2.20
2 c	-10.09	2 c	7.18	2 c	32.57
3 c	-30.22	3 c	8.28	3 c	32.51
4 c	-26.45	4 c	-17.28	4 c	1.83
5 cu	-167.43	5 cu	333.25	5 cu	270.89
6 cu	-141.00	6 cu	330.99	6 cu	269.99
7 c	-20.10	7 c	-16.06	7 c	4.08
8 c	-68.07	8 c	-25.77	8 c	3.54
9 c	4.53	9 c	6.78	9 c	31.93
10 c	-40.81	10 c	7.30	10 c	31.92
11 si	323.18	11 si	329.01	11 si	328.61
12 si	329.33	12 si	330.04	12 si	328.85
13 si	328.83	13 si	328.47	13 si	328.24
14 si	331.96	14 si	329.54	14 si	327.80
		93 li	88.99	93 li	93.93
		94 li	88.93	94 li	93.92
				95 li	93.84
				96 li	93.85

4 Cu – Cu distances

Table 25 Distances between the copper atoms in the investigated molecules in Å. In addition, the van der Waals radius,¹ the covalent radius based on crystallographic studies on a large number of copper compounds,² as well as the covalent radius for single Cu – Cu bonds³ are listed for comparison.

Molecule	Distance, [Å]
A_0	2.53
A_2	2.78
A_4	2.65
B_0	2.38
B_2	2.36
B_4	2.46
van der Waals radius	1.4
covalent radius	1.32(4)
covalent radius (single bond)	1.12

5 Visual representations of the current densities.

The LIC representations of the current densities at varying distance from the molecular plane for the investigated molecules.

5.1 Naphthalene

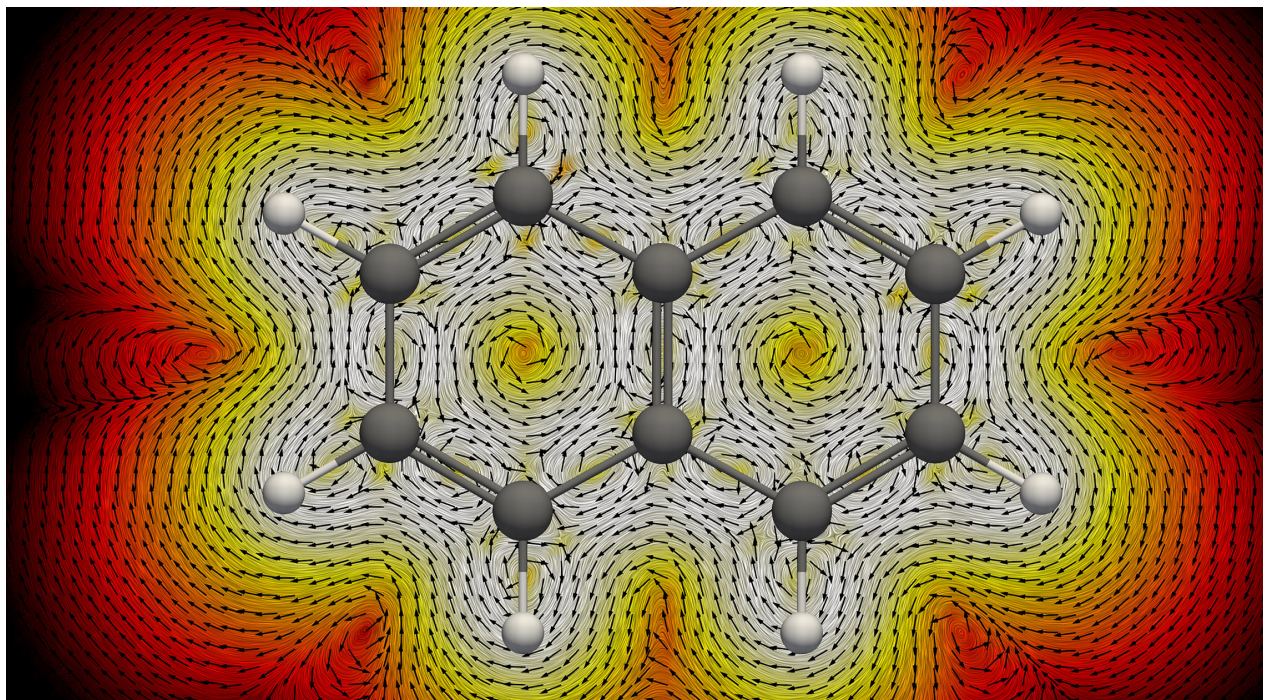


Fig. 1 LIC representation of the current density in the molecular plane of naphthalene.

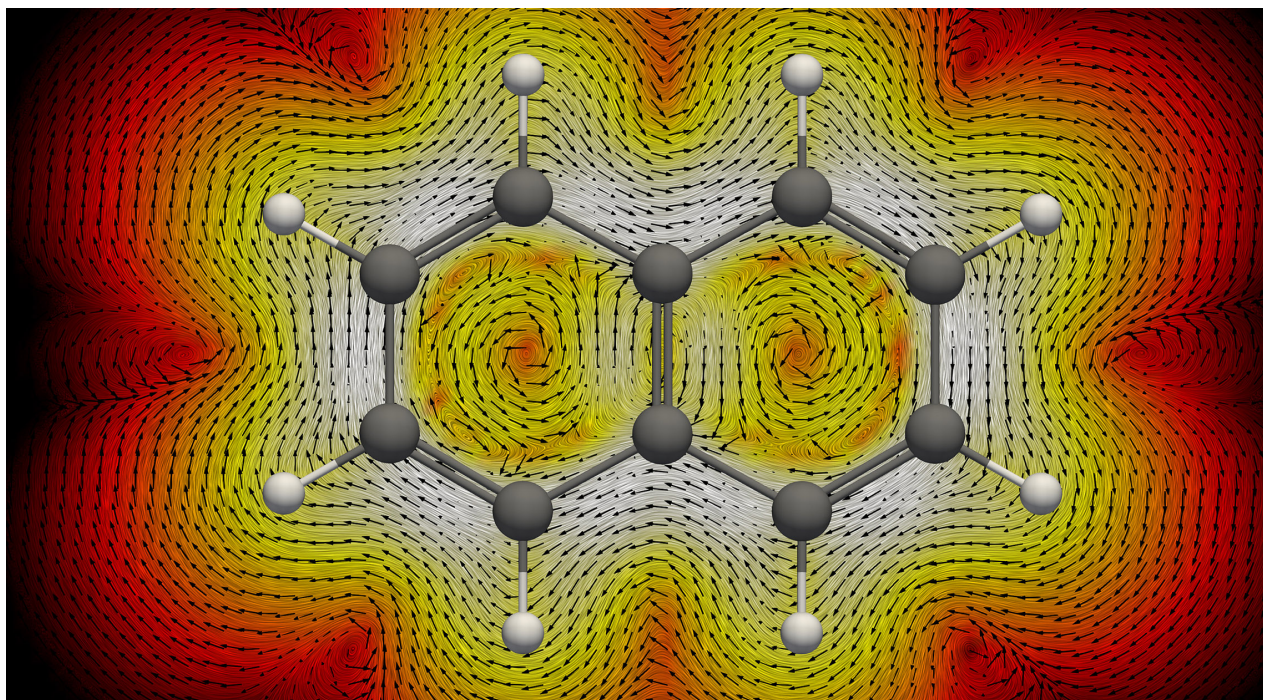


Fig. 2 LIC representation of the current density 1.0 bohr from the molecular plane of naphthalene.

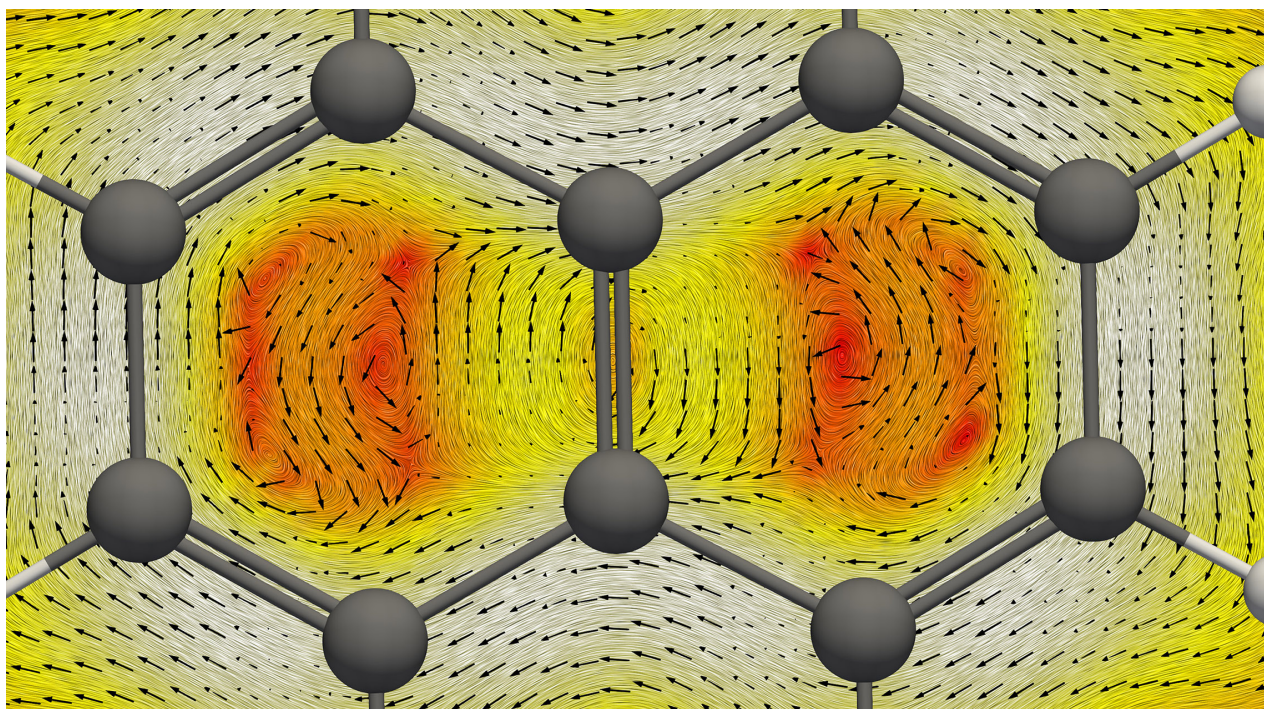


Fig. 3 LIC representation of the current density 1.5 bohr from the molecular plane of naphthalene.

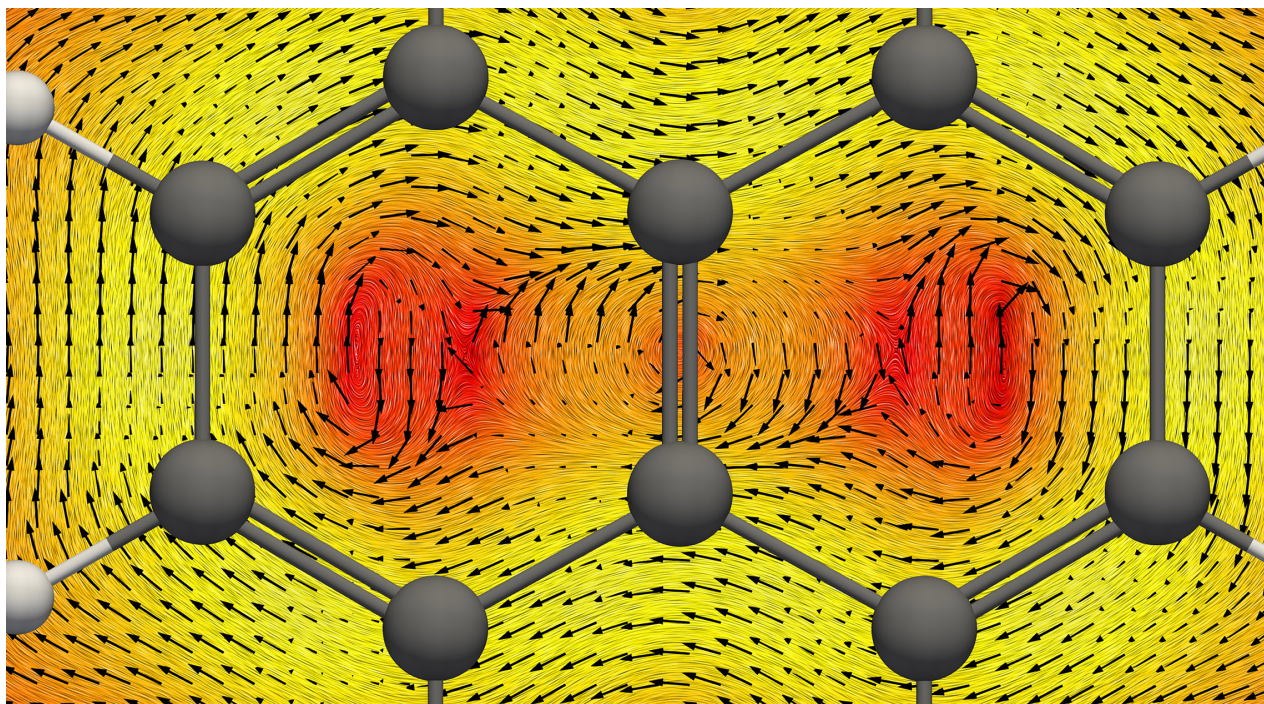


Fig. 4 LIC representation of the current density 2.0 bohr from the molecular plane of naphthalene.

5.2 [10]annulene in heart-shaped conformation

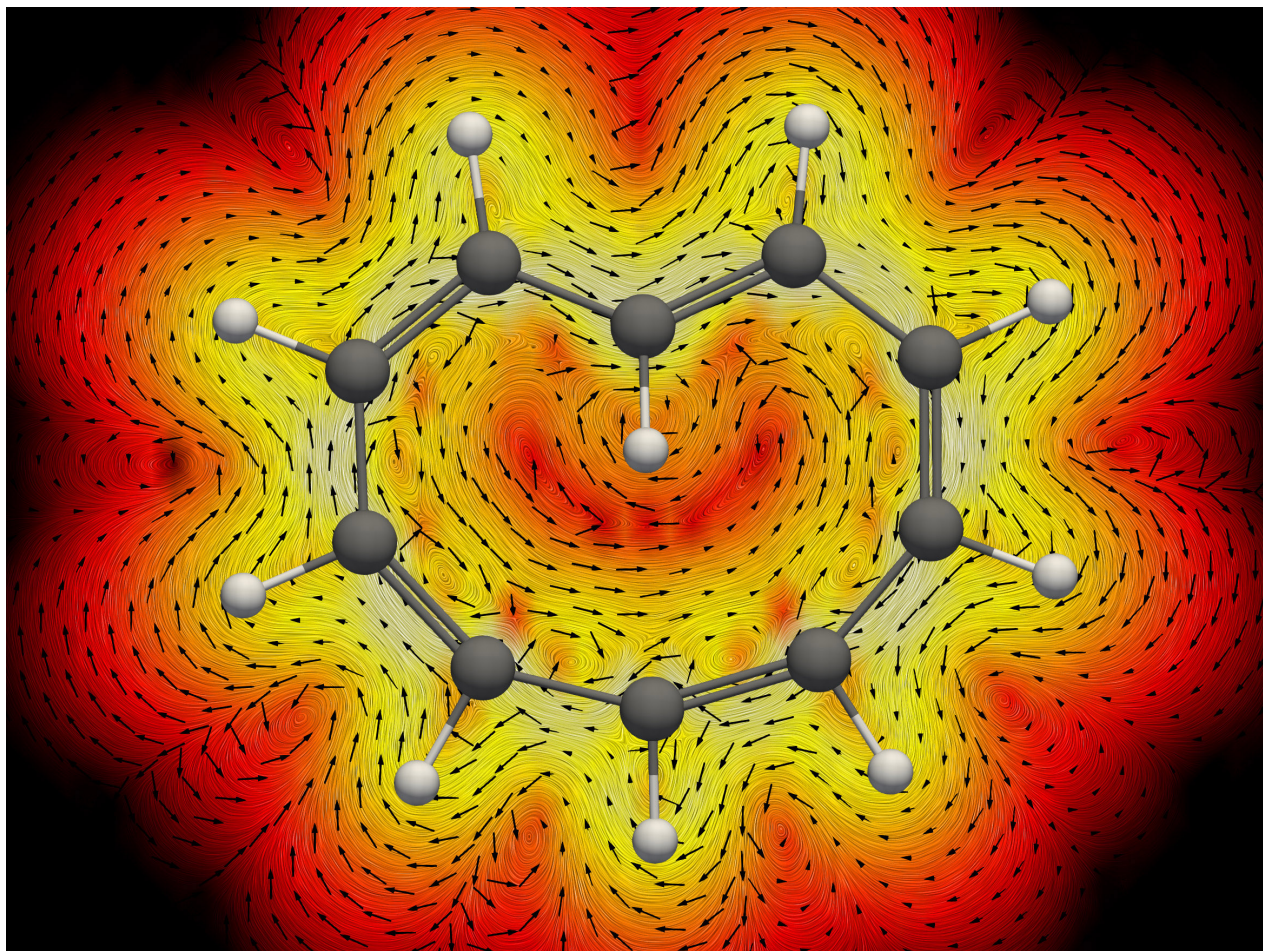


Fig. 5 LIC representation of the current density 0.5 bohr above the base plane in the heart-shaped conformation of [10]annulene.

5.3 [10]annulene in all-*cis* conformation

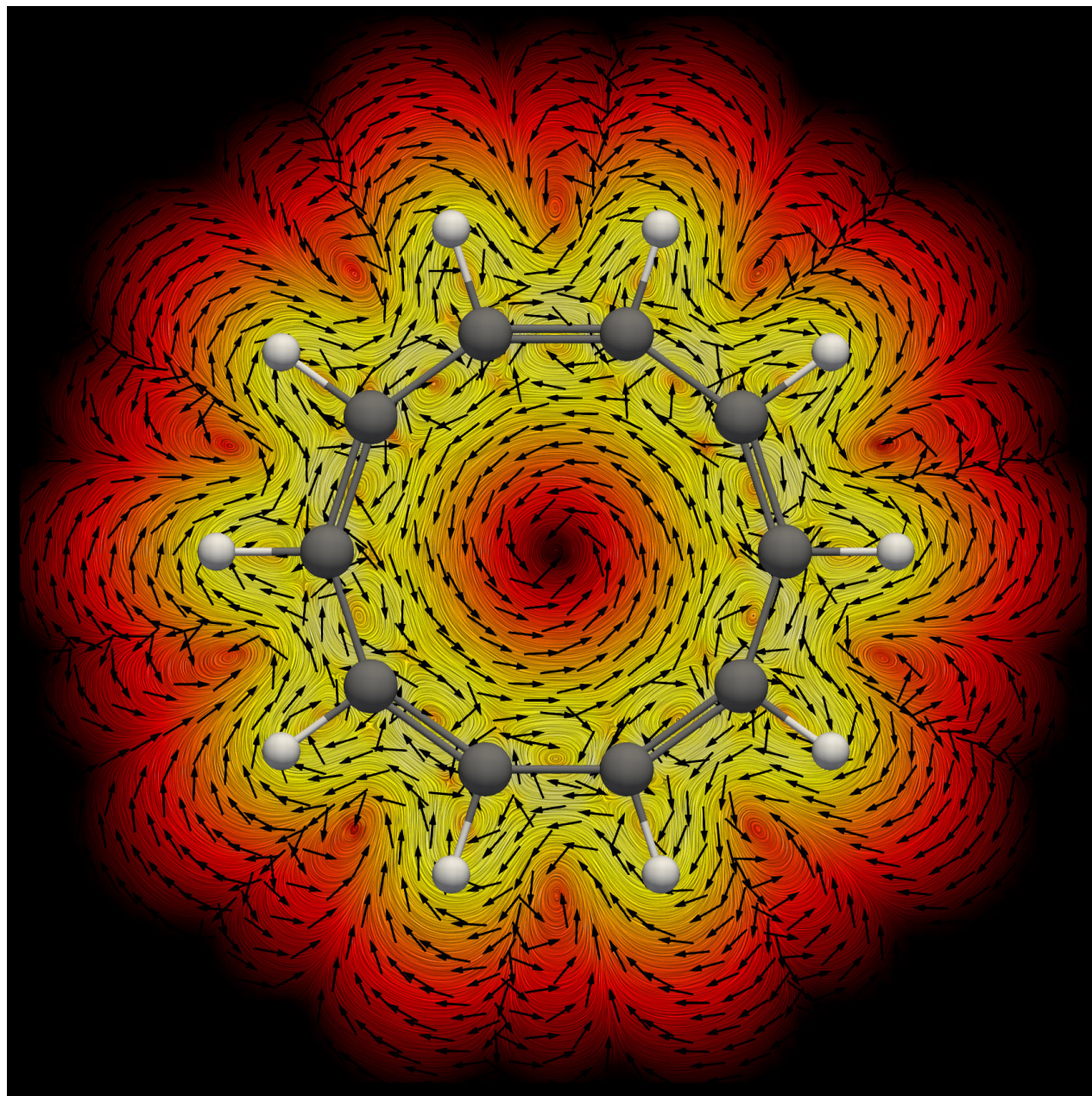


Fig. 6 LIC representation of the current density in the molecular plane in the all-*cis* conformation of [10]annulene.

5.4 [10]annulene in all-*trans* conformation

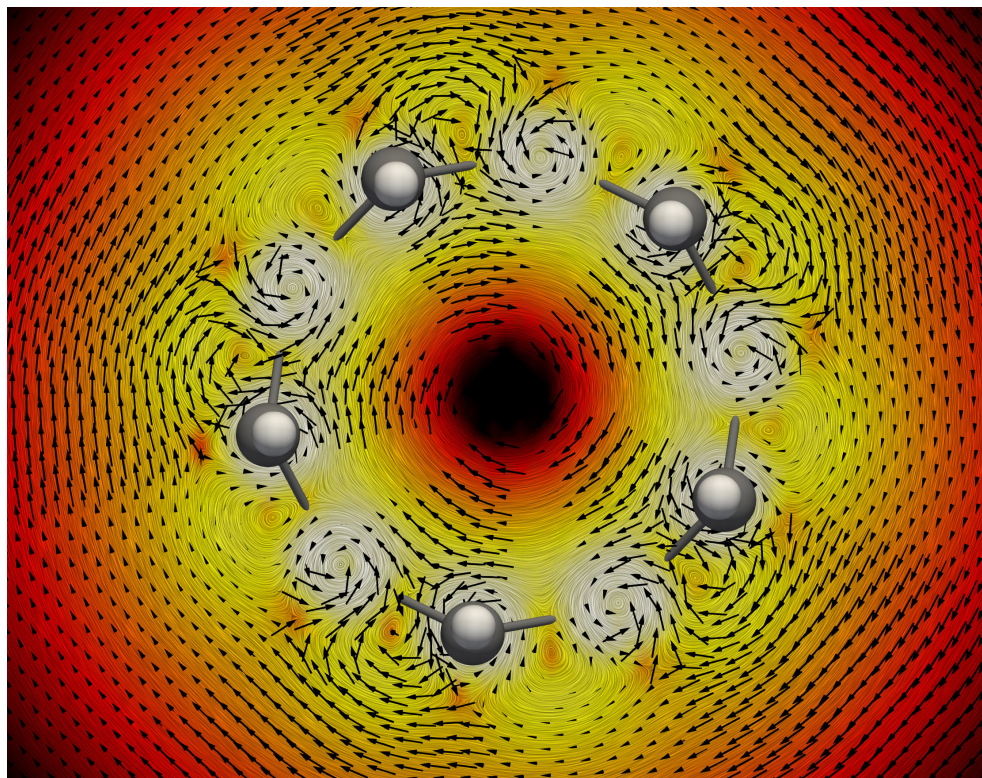


Fig. 7 LIC representation of the current density in the base plane in the all-*trans* conformation of [10]annulene.

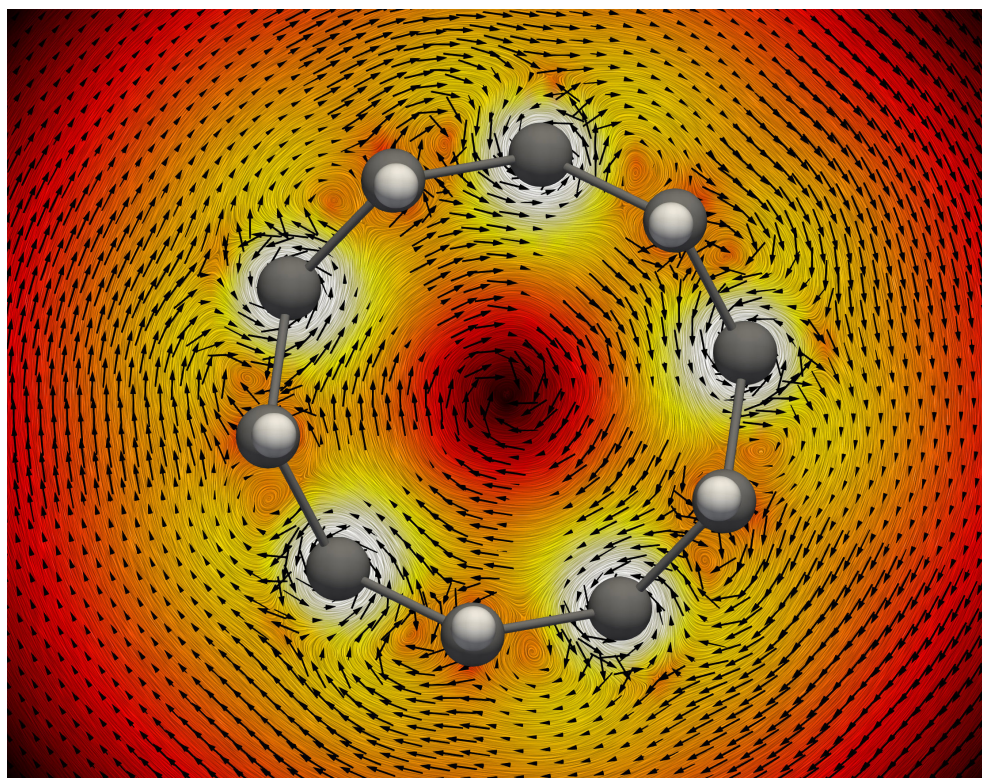


Fig. 8 LIC representation of the current density 1 bohr above the base plane in the all-*trans* conformation of [10]annulene.

5.5 Molecule A_0

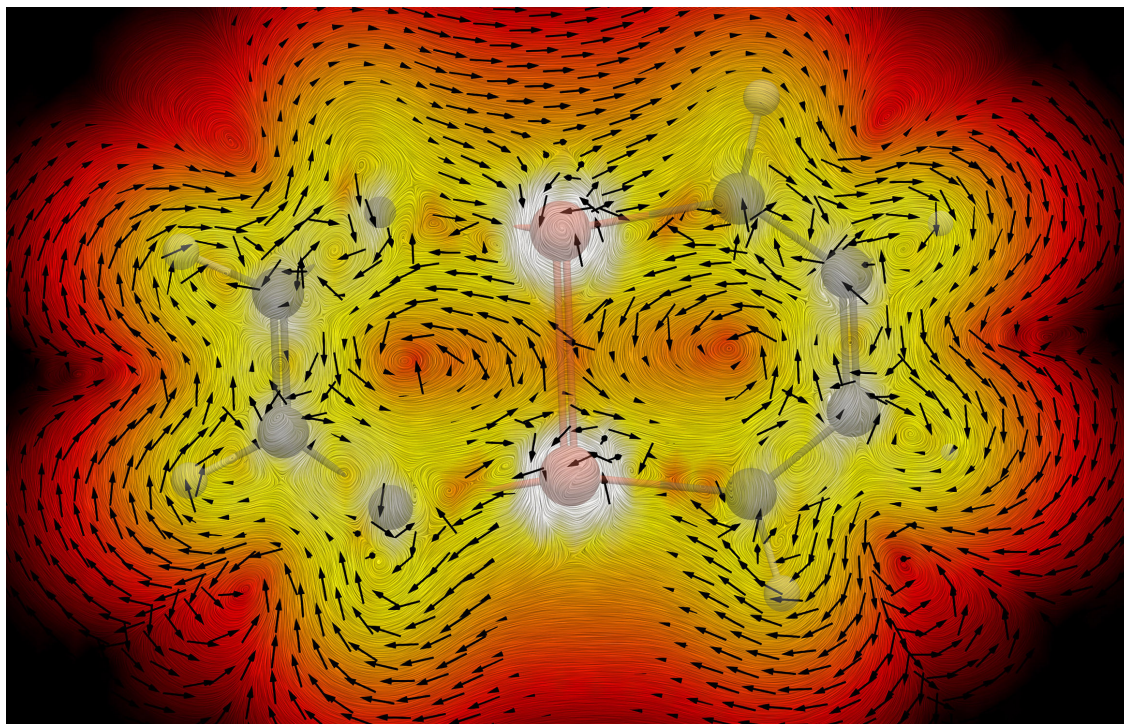


Fig. 9 LIC representation of the current density in the base plane of molecule A_0 .

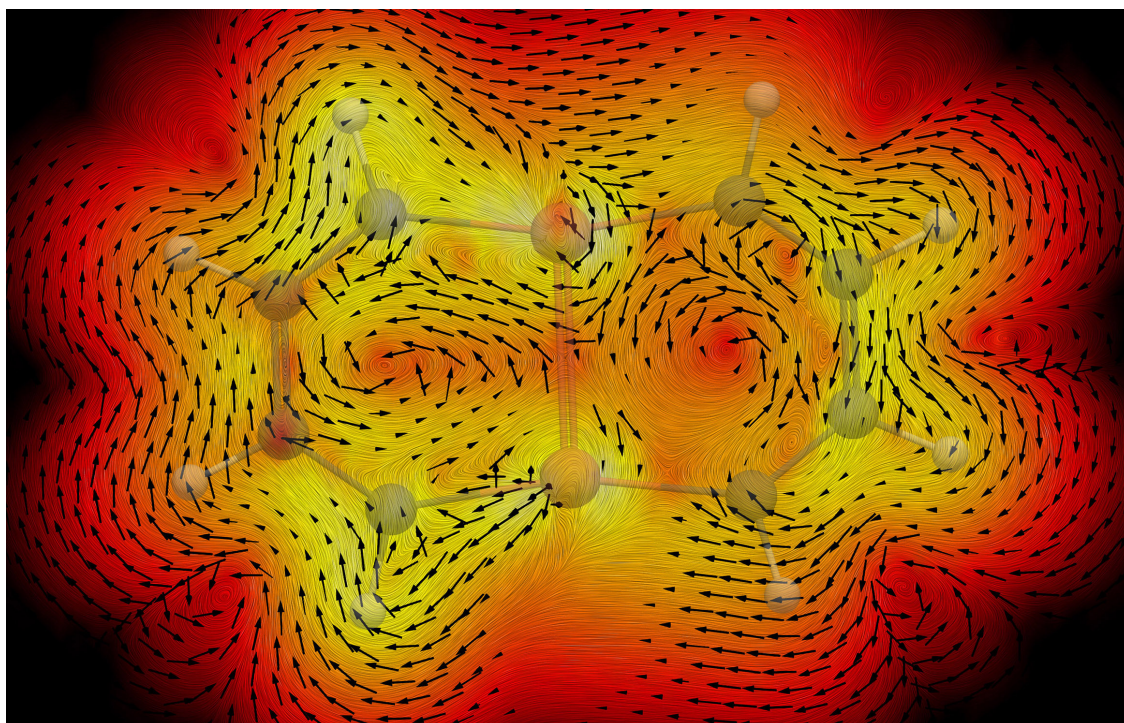


Fig. 10 LIC representation of the current density 1.0 bohr from the base plane of molecule A_0 .

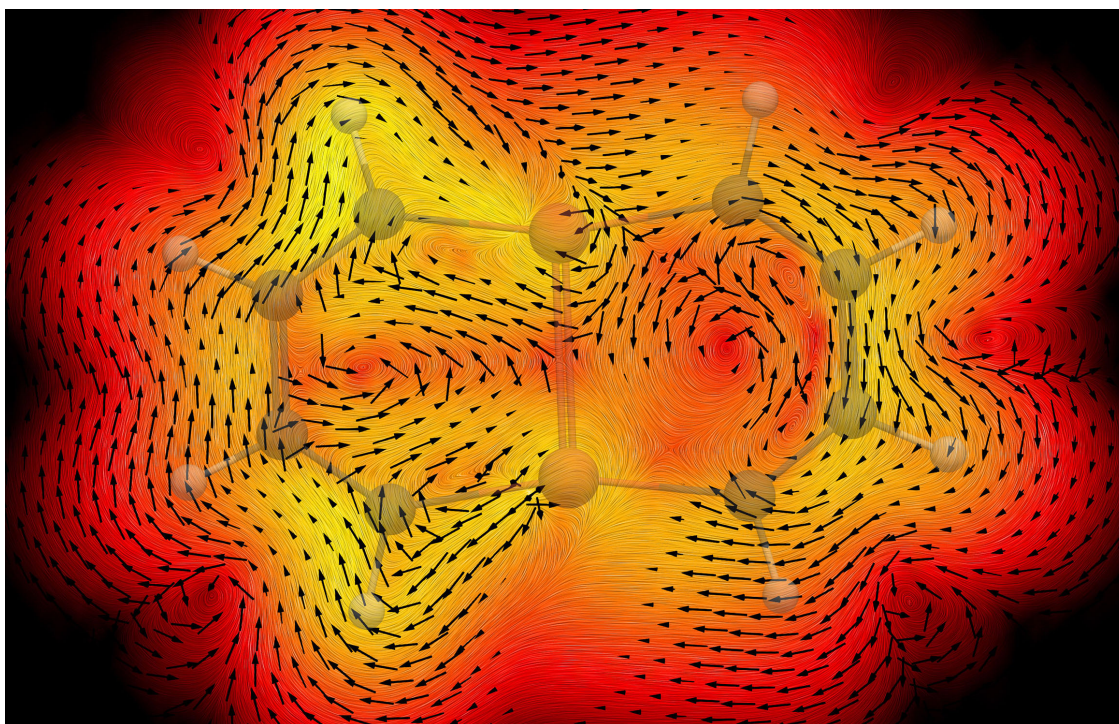


Fig. 11 LIC representation of the current density 1.5 bohr from the base plane of molecule A_0 .

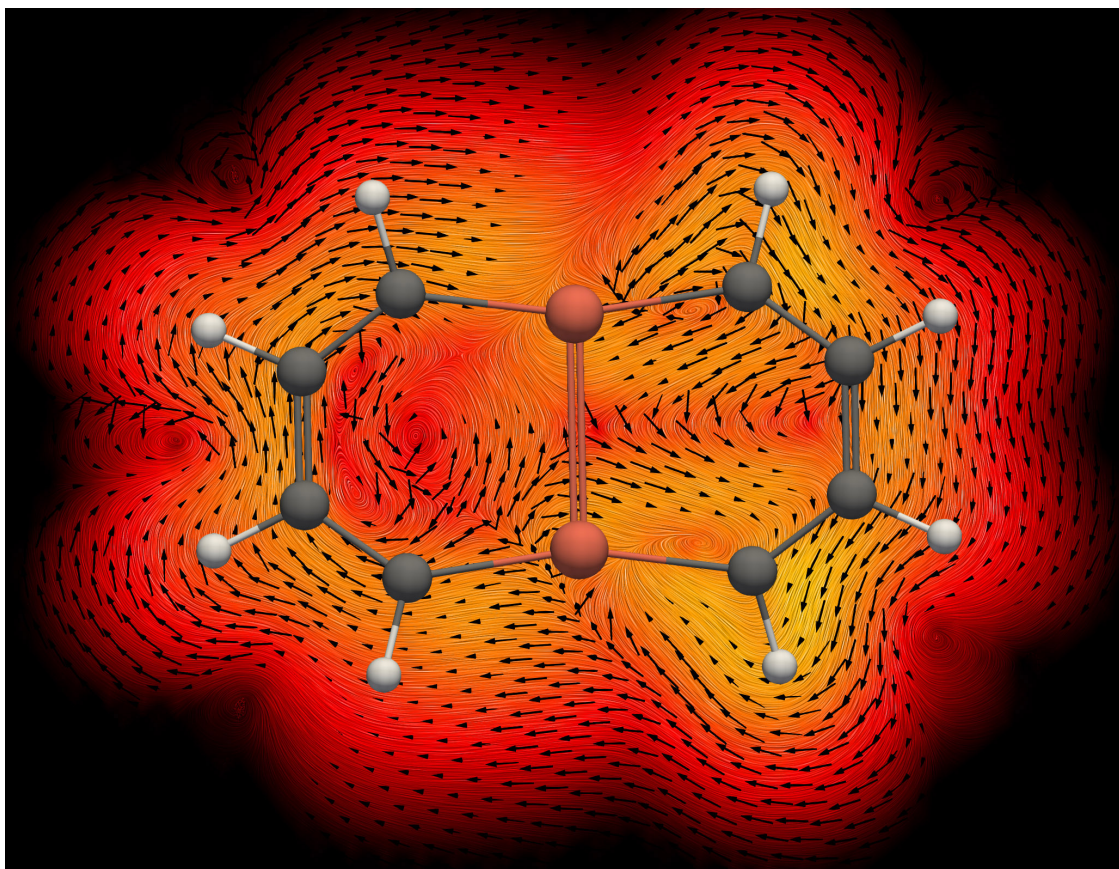


Fig. 12 LIC representation of the current density 2.0 bohr from the base plane of molecule A_0 .

5.6 Molecule A_2

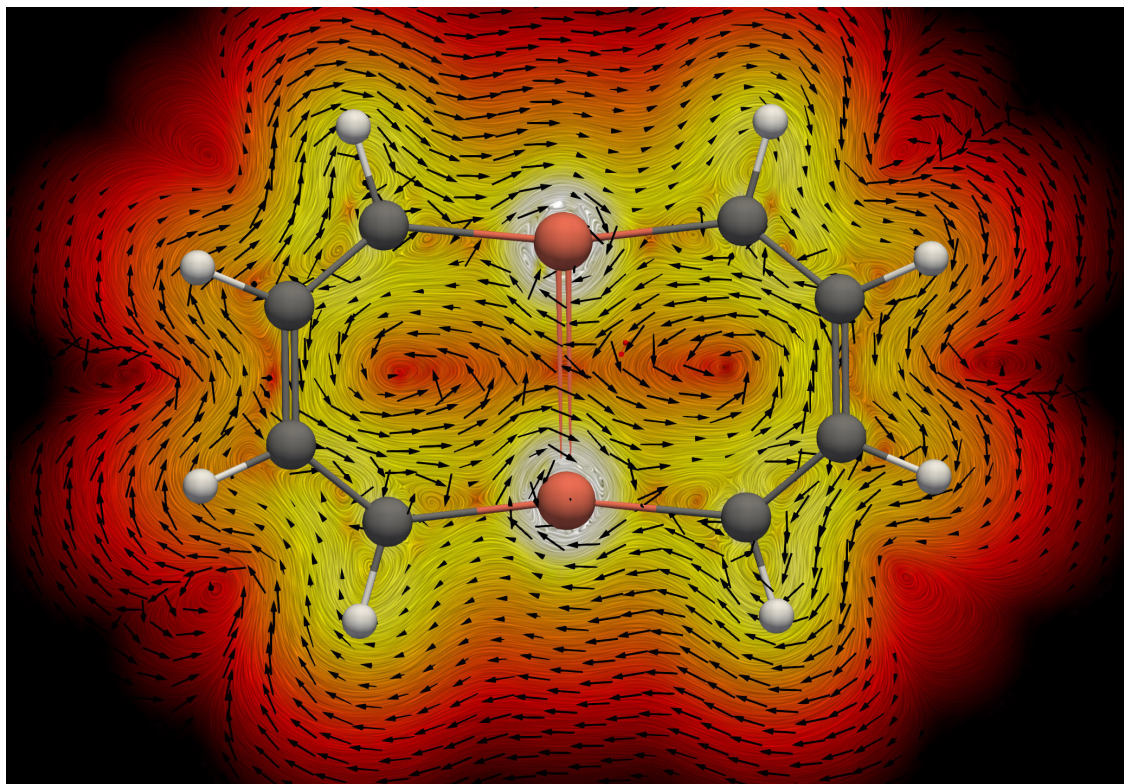


Fig. 13 LIC representation of the current density in the base plane of molecule A_2 .

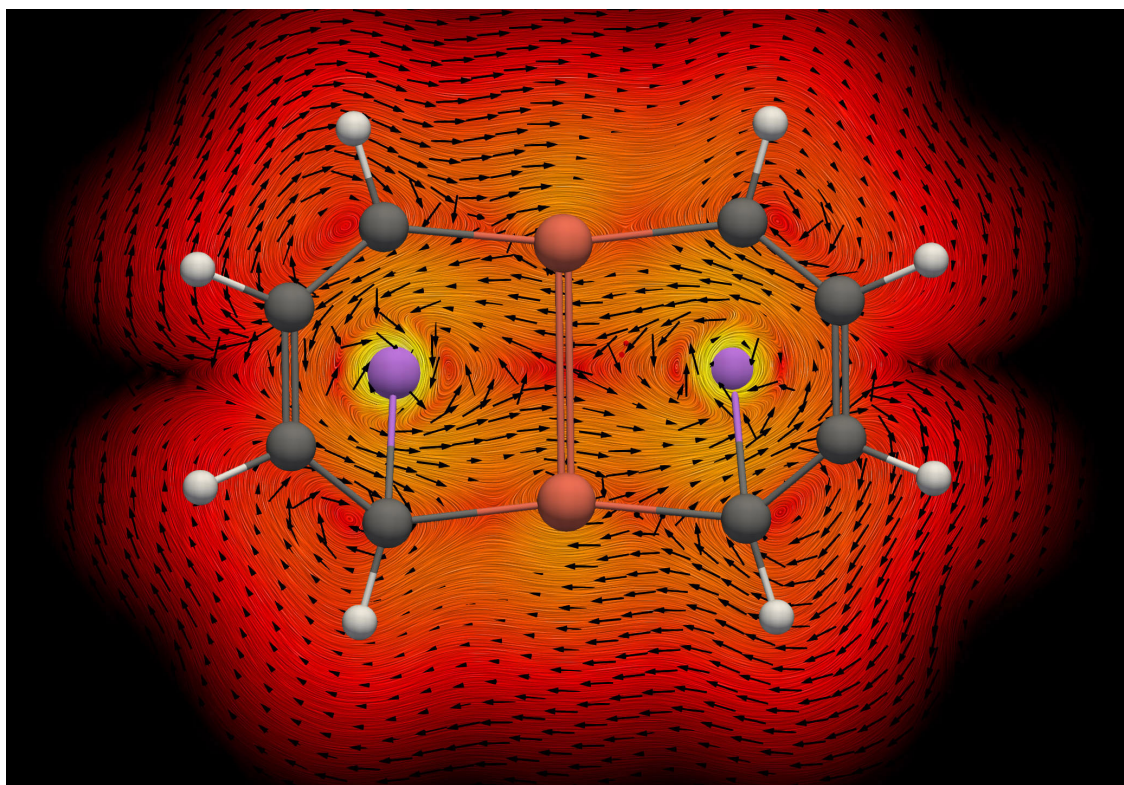


Fig. 14 LIC representation of the current density 2.0 bohr from the base plane of molecule A_2 .

5.7 Molecule A_4

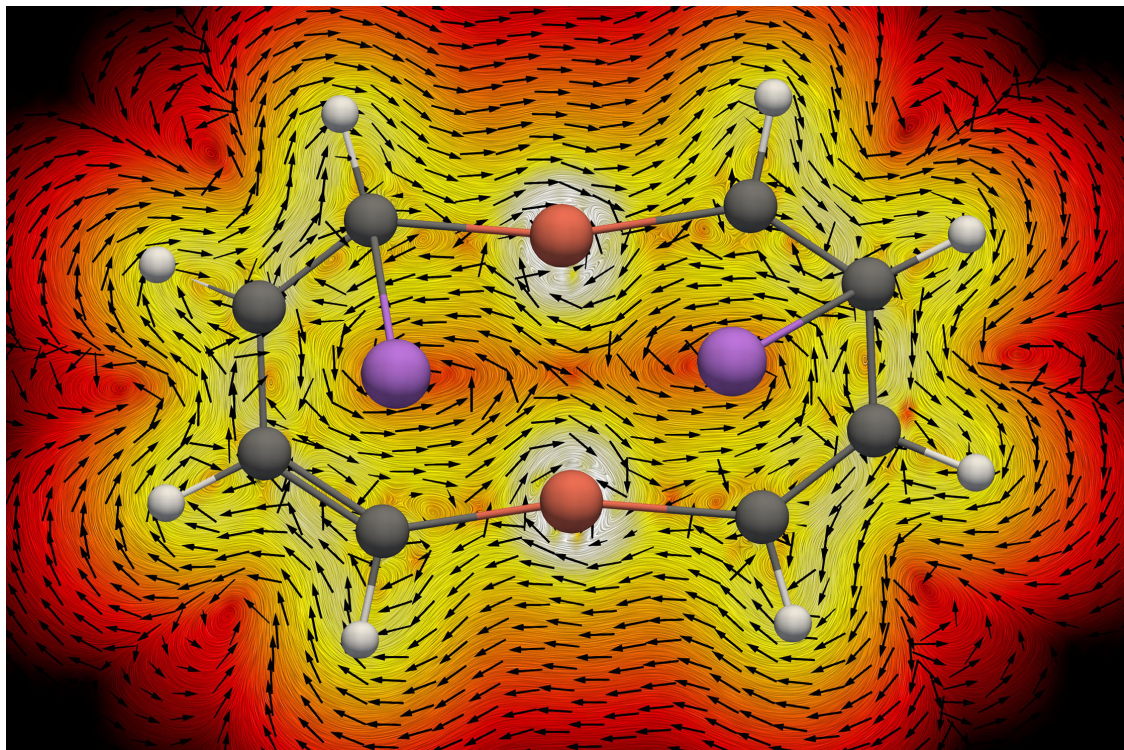


Fig. 15 LIC representation of the current density in the molecular plane of molecule A_4 .

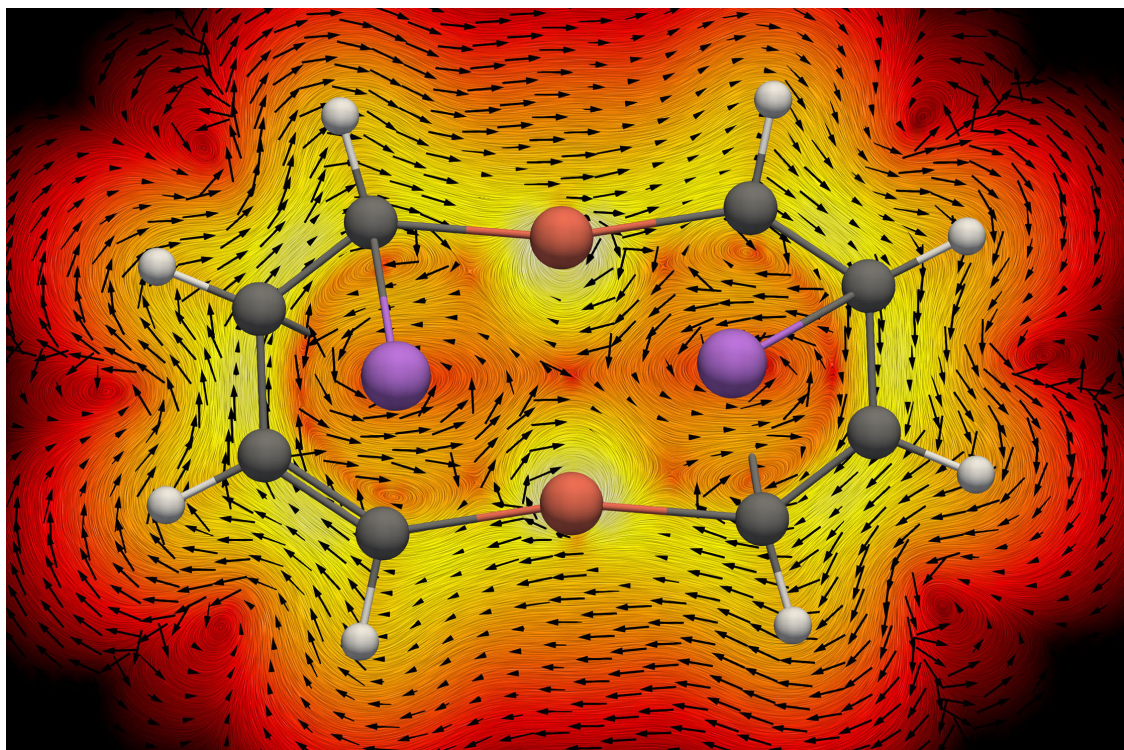


Fig. 16 LIC representation of the current density 1.0 bohr from the molecular plane of molecule A_4 .

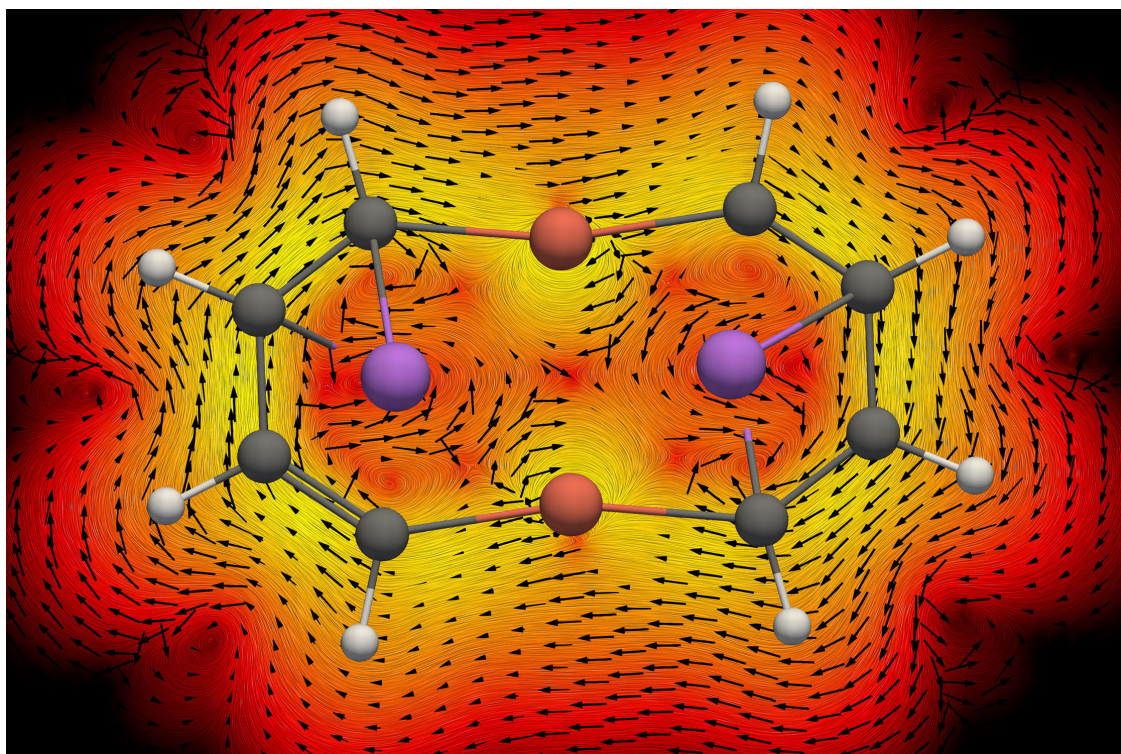


Fig. 17 LIC representation of the current density 1.5 bohr from the molecular plane of molecule **A₄**.

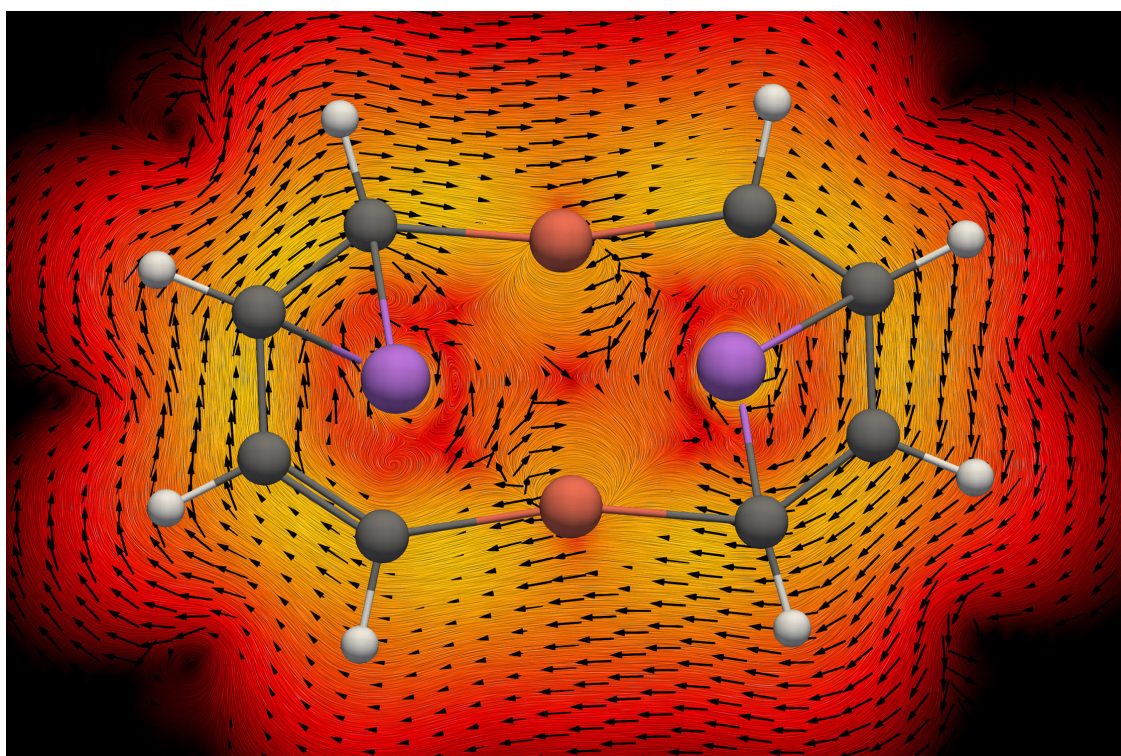


Fig. 18 LIC representation of the current density 2.0 bohr from the molecular plane of molecule **A₄**.

5.8 Molecule B₄

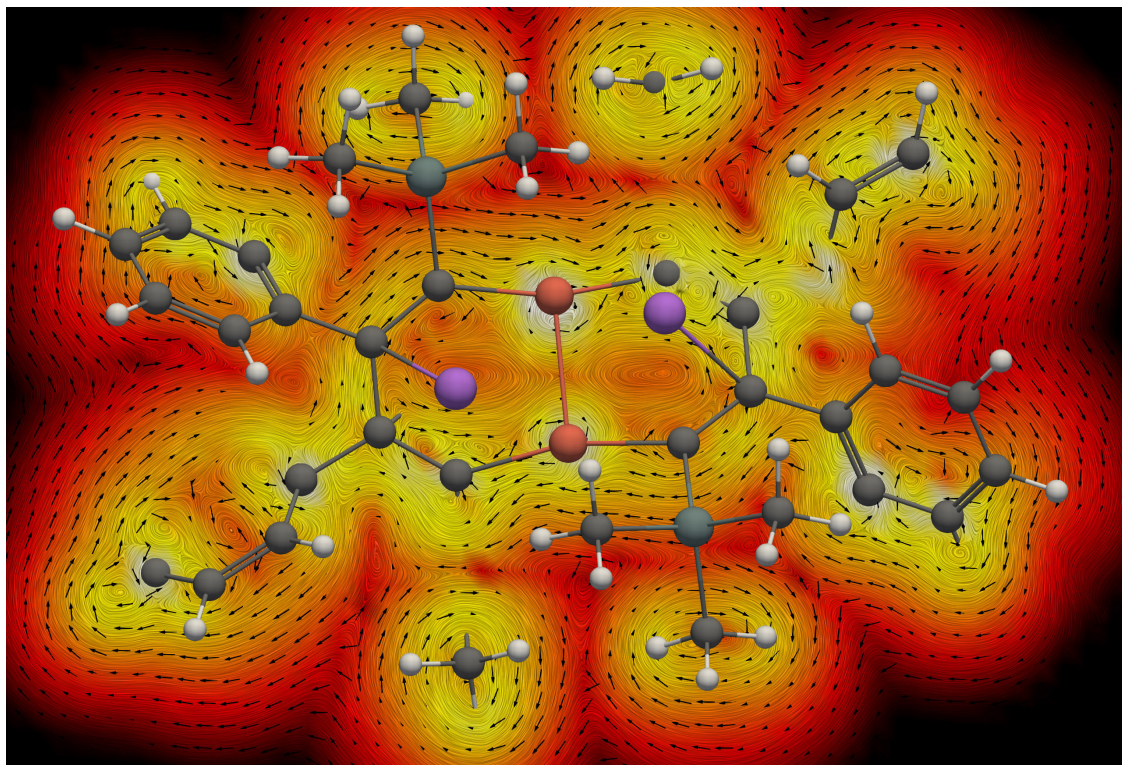


Fig. 19 LIC representation of the current density in the base plane of molecule **B₄**.

5.9 Close-up view on the current densities between the two copper atoms

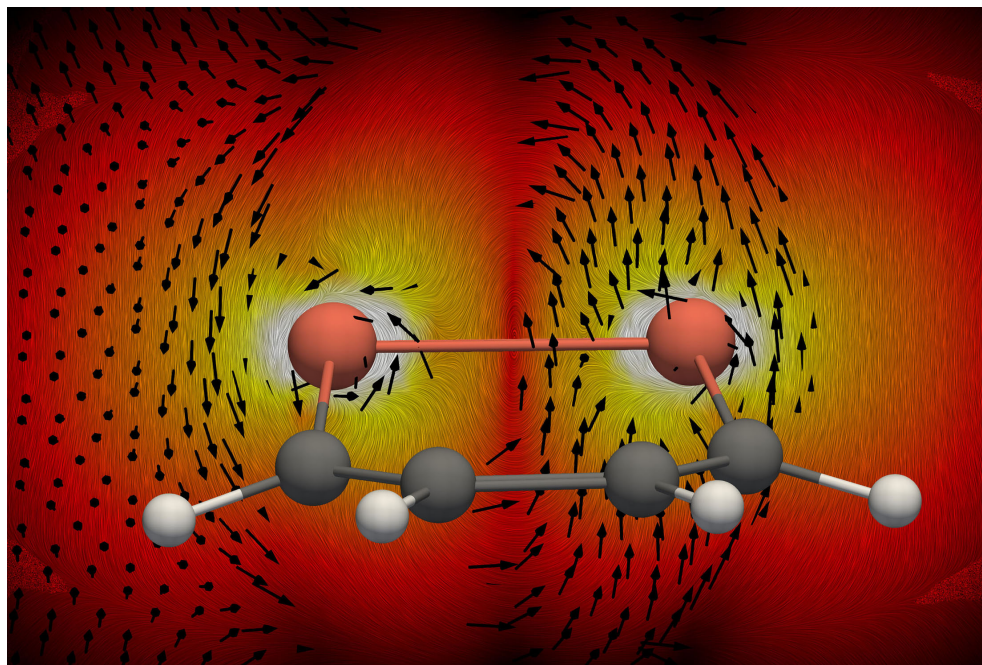


Fig. 20 LIC representation of the current density between the copper atoms in molecule A_0 .

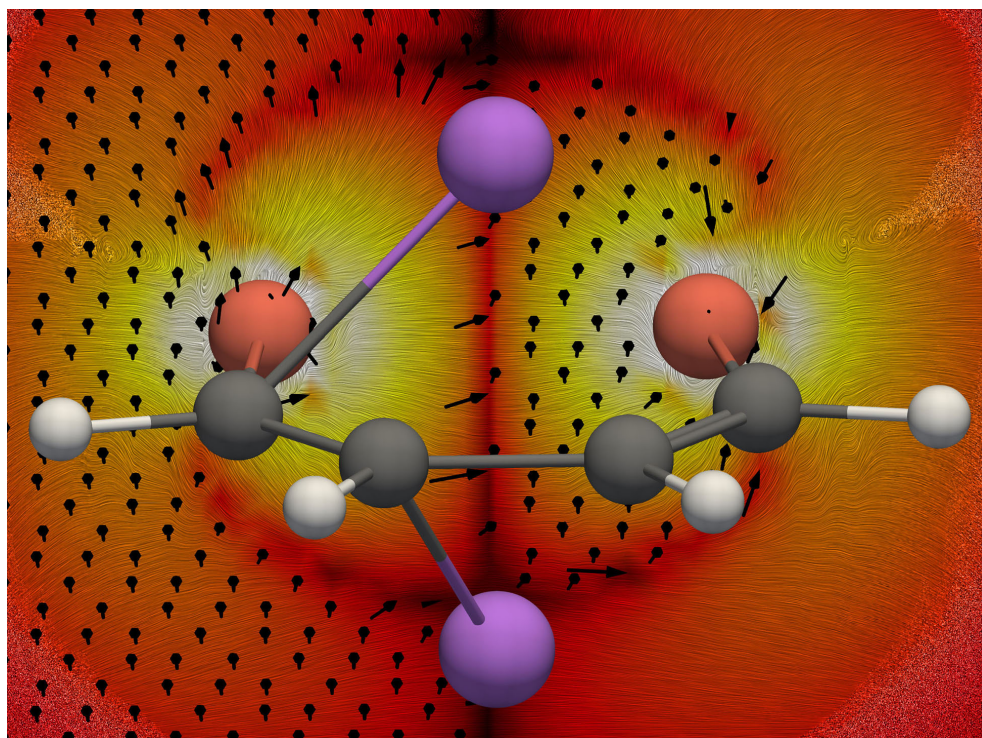


Fig. 21 LIC representation of the current density between the copper atoms in molecule A_4 .

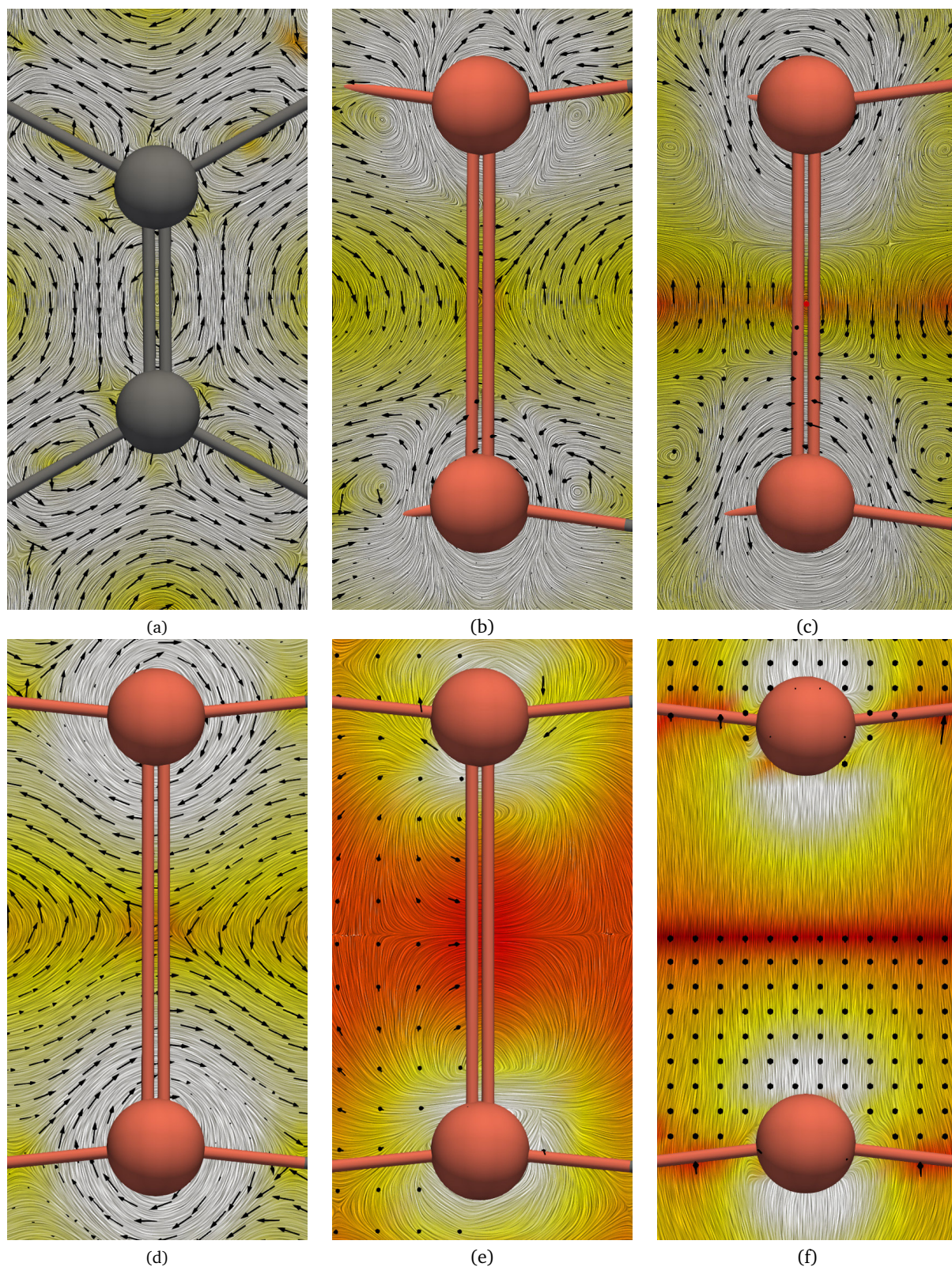


Fig. 22 Comparison of the induced bond currents of the common bond between the two rings in the molecular plane. The orientation of the external magnetic field is marked as $B_{ext}^{\parallel}$ if it lies in the molecular plane and it is perpendicular to the investigated bond, and as $B_{ext}^{\perp}$ if it is normal to the molecular plane. (a) naphthalene, $B_{ext}^{\perp}$; (b) dicupra[10]annulene without substituents ($\mathbf{A}_0$), $B_{ext}^{\perp}$; (c) dicupra[10]annulene without substituents ($\mathbf{A}_0$), $B_{ext}^{\parallel}$; (d) dicupra[10]annulene without substituents and two lithium ions ($\mathbf{A}_2$), $B_{ext}^{\perp}$; (e) dicupra[10]annulene without substituents and two lithium ions ($\mathbf{A}_2$), $B_{ext}^{\parallel}$; (f) dicupra[10]annulene without substituents and four lithium ions ($\mathbf{A}_4$), $B_{ext}^{\parallel}$. The vortices in between the copper atoms in (c) and (e) are cross-sections of vertically oriented currents, rather than bond currents based on the thorough analysis of the current flow in the molecules.

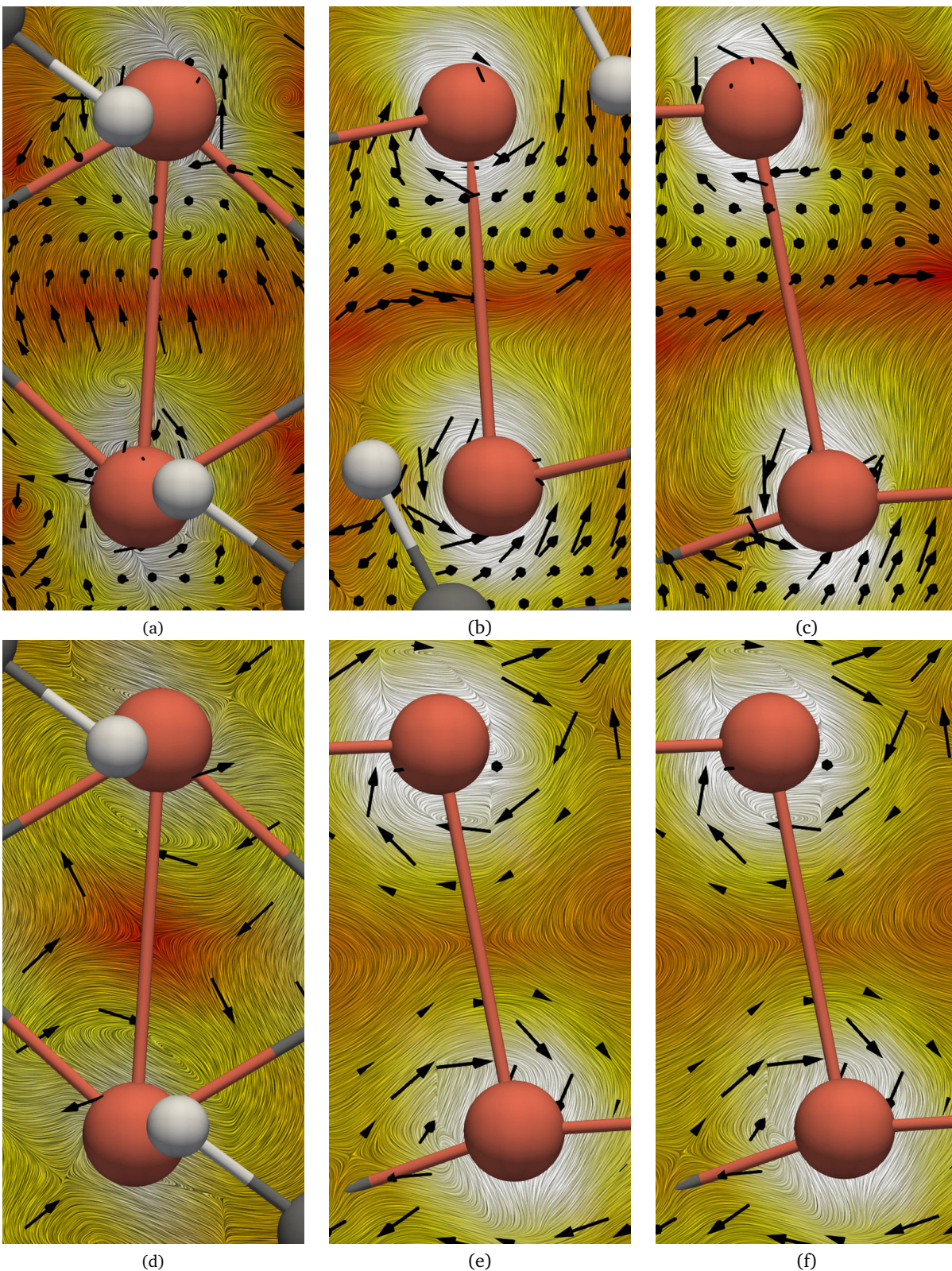


Fig. 23 Comparison of the induced bond currents of the common bond between the two rings in the molecular plane in the substituted molecules. The orientation of the external magnetic field is marked as $B_{ext}^{\parallel}$ if it lies in the molecular plane and it is perpendicular to the investigated bond, and as $B_{ext}^{\perp}$ if it is normal to the molecular plane. (a) dicupra[10]annulene with substituents and no lithium ions ($\mathbf{B}_0$), $B_{ext}^{\parallel}$; (b) dicupra[10]annulene with substituents and two lithium ions ($\mathbf{B}_2$), $B_{ext}^{\perp}$; (c) dicupra[10]annulene with substituents and four lithium ions ($\mathbf{B}_4$), $B_{ext}^{\perp}$; (d) dicupra[10]annulene with substituents and no lithium ions ($\mathbf{B}_0$), $B_{ext}^{\parallel}$; (e) dicupra[10]annulene without substituents and two lithium ions ($\mathbf{B}_2$), $B_{ext}^{\parallel}$; (f) dicupra[10]annulene without substituents and four lithium ions ($\mathbf{B}_4$), $B_{ext}^{\parallel}$

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