Most Favorable Cumulenic Structures in Iron-Capped Linear Carbon Chains are Short Singlet Odd-Carbon Dications: A Theoretical View

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Electronic Supplementary Information

spin-flip DFT (SF-DFT) method (non-collinear SF-DFT with PBE0/6-31+G*).

Table S3. Bond distances (Å) of $[FeC_nFe]^{2+}$ chains from one end to another for iron-capped linear carbon dications in singlet and triplet states. Fe−C bond shown in red.

Table S4. Mayer bond order between adjacent atoms in the chain from one end to another for iron-capped linear carbon dications $[FeC_nFe]^{2+}$ in singlet and triplet states.

Tables S5-54. Theoretical Cartesian coordinates for all complexes. (see the txt ESI file)

Complete Gaussian reference (reference 78)

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Computational Details

The linear structures exhibit convergence problems during the geometry optimizations using Gaussian 09. Generally, an optimization job started with the default optimizing method, namely GEDIIS. If this job cannot converge in 60 cycles, it continued using GDIIS method. In some cases, using both GEDIIS and GDIIS methods cannot guarantee convergence, then RFO method was performed. The initial structure was built upon a shorter optimized one without imposing any symmetry. However during all optimization jobs, the additional keyword symm=loose was used. All convergence criteria, the SCF process and the optimization, utilized the default values of Gaussian 09. Following each optimization the harmonic vibrational frequencies were evaluated to confirm local minima and to obtain thermodynamic data.

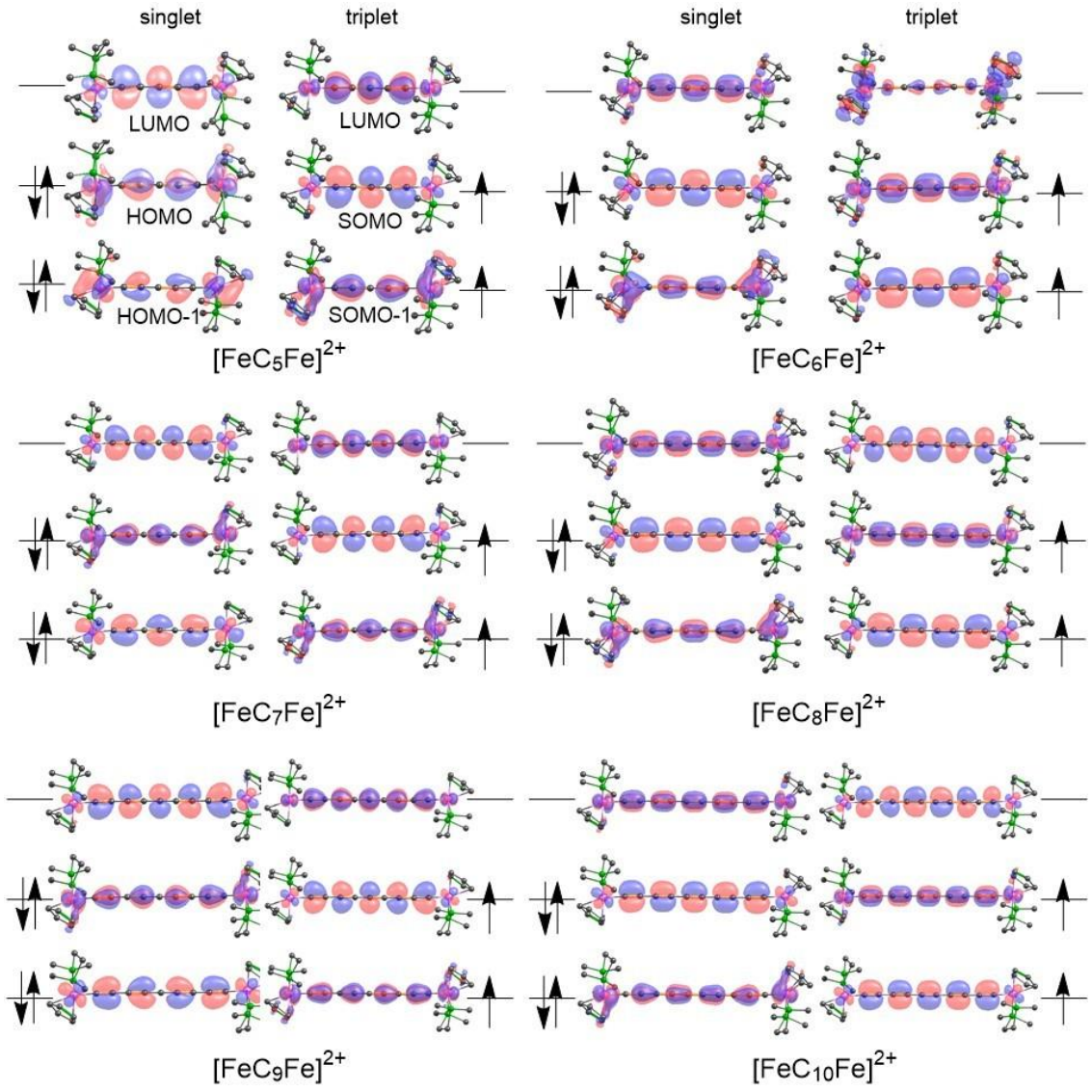

Figure S1. The highest occupied molecular orbitals (HOMO), HOMO−1, the singly occupied molecular orbital (SOMO), SOMO−1 and the lowest unoccupied molecular orbitals (LUMO) from $[FeC_5Fe]^{2+}$ to $[FeC_{10}Fe]^{2+}$ in singlet and triplet states.

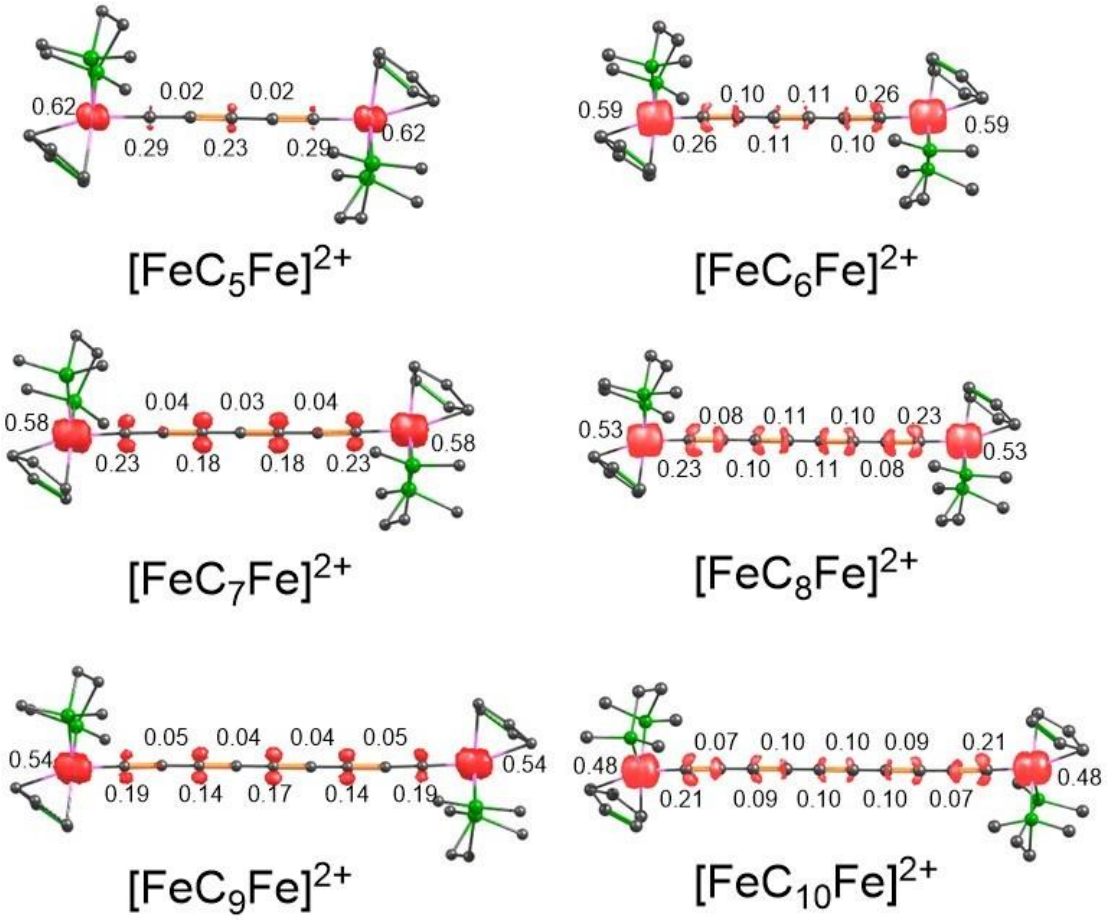

Figure S2. Spin densities in complexes from $[FeC_5Fe]^{2+}$ to $[FeC_{10}Fe]^{2+}$ in triplet states.

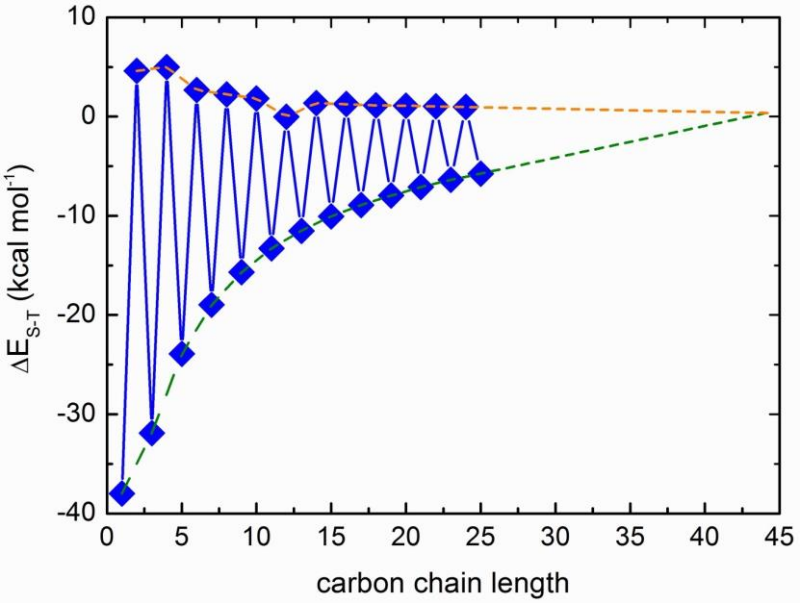

Figure S3. Singlet-triplet energy splittings (electronic energies with ZPVE correction) for the iron-capped carbon chains and extrapolation for odd- and even-chains.

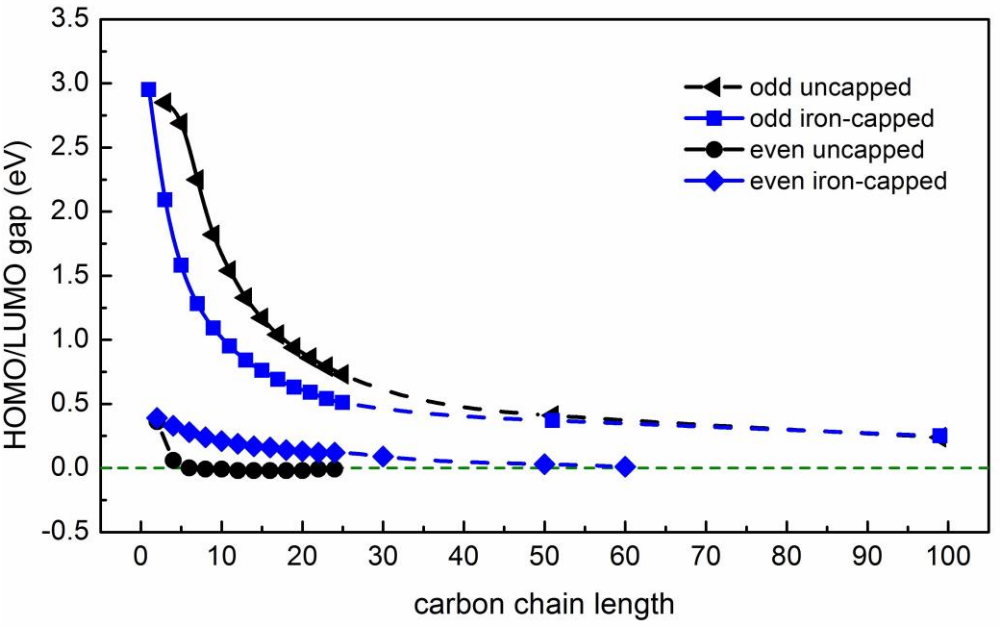

Figure S4. HOMO/LUMO gaps for the iron-capped and uncapped carbon chains with extrapolations.

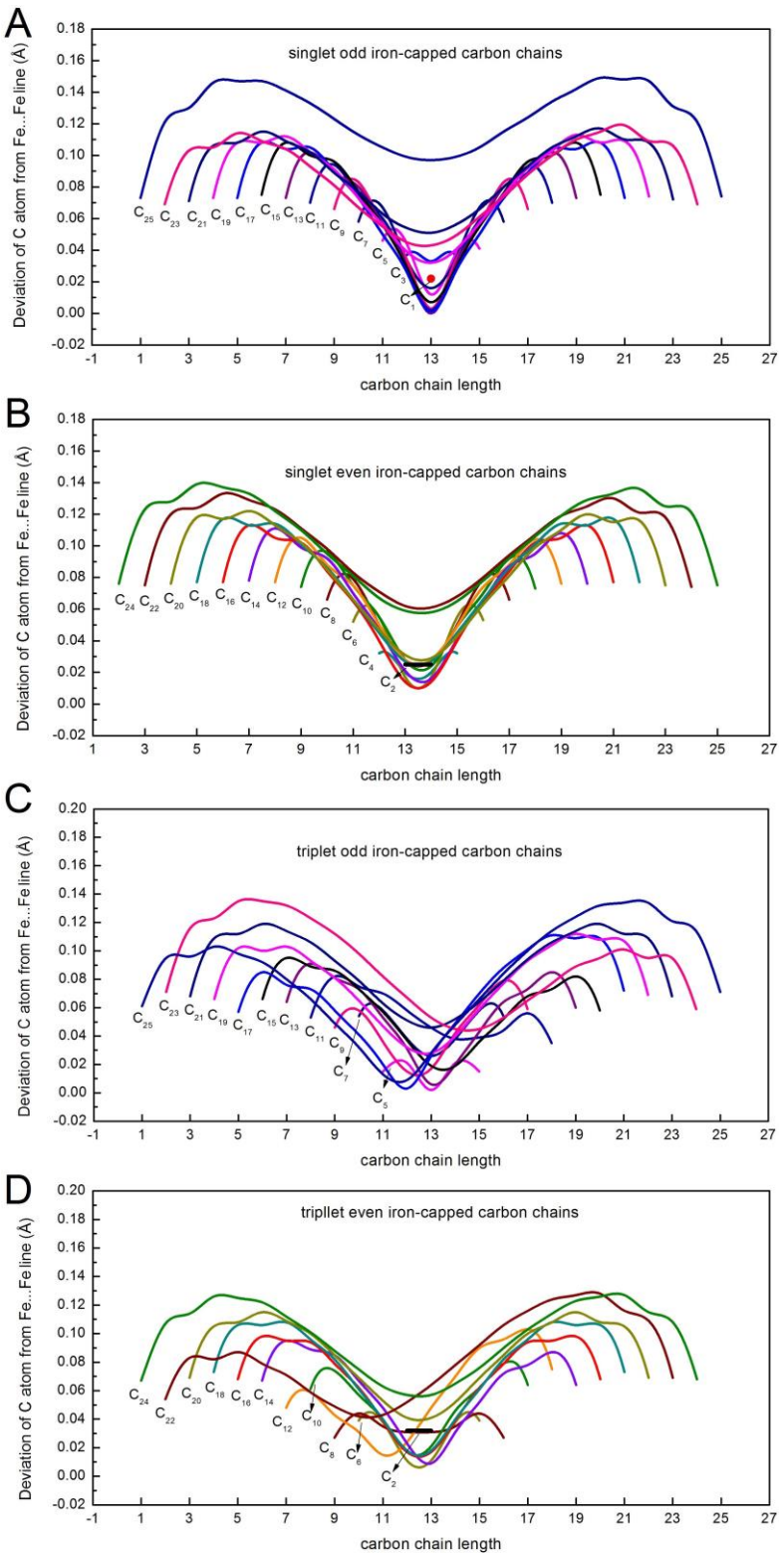

Figure S5. Deviation of carbon atoms from Fe···Fe line. A and B: singlet odd and even $[FeC_nFe]^{2+}$ chains; C and D: triplet odd and even $[FeC_nFe]^{2+}$ chains.

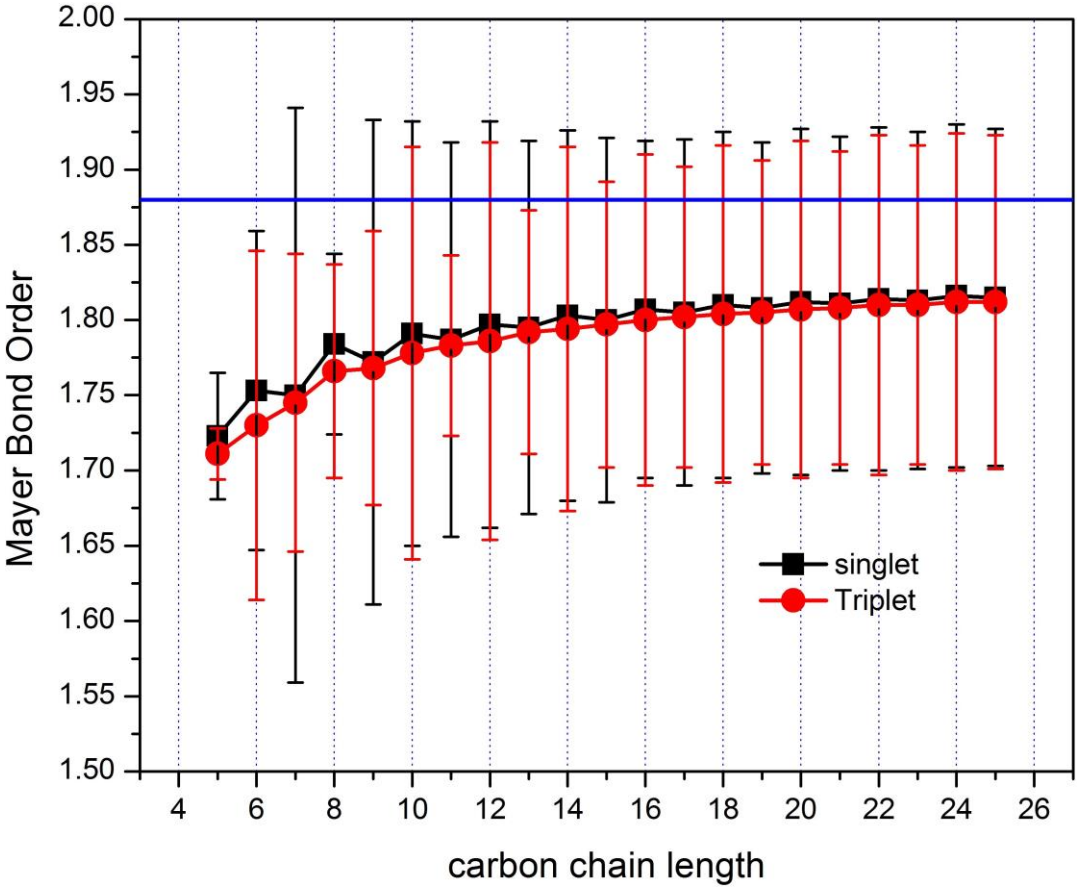

Figure S6. Average C−C Mayer bond orders (MBO) and MBO ranges of the iron-capped linear carbon dications $[FeC_nFe]^{2+}$ in singlet and triplet states. Blue line: C−C MBO of allene.

Table S1. Electronic energies with zero-point vibrational energy corrections for odd and even iron-capped linear carbon dications, all in singlet and triplet states.

Odd carbon chain				Even carbon chain			
n_C	E(S)/hartree	E(T)/hartree	ΔE(S−T) Kcal mol^{-1}	n_C	E(S)/hartree	E(T)/hartree	ΔE(S−T) Kcal mol^{-1}
1	−4793.543693	−4793.483161	−37.98	2	−4831.610518	−4831.617881	4.62
3	−4869.721057	−4869.670202	−31.91	4	−4907.775872	−4907.783825	4.99
5	−4945.878829	−4945.840712	−23.92	6	−4983.938100	−4983.942356	2.67
7	−5022.035030	−5022.004799	−18.97	8	−5060.096506	−5060.100084	2.25
9	−5098.189641	−5098.164661	−15.68	10	−5136.252947	−5136.255867	1.83
11	−5174.343411	−5174.322241	−13.28	12	−5212.408156	−5212.408104	−0.03
13	−5250.496657	−5250.478318	−11.51	14	−5288.562687	−5288.564869	1.37
15	−5326.649533	−5326.633528	−10.04	16	−5364.71646	−5364.718472	1.26
17	−5402.802148	−5402.787948	−8.91	18	−5440.86982	−5440.871614	1.13
19	−5478.954496	−5478.941805	−7.96	20	−5517.022805	−5517.024564	1.10
21	−5555.106635	−5555.095316	−7.10	22	−5593.175502	−5593.177147	1.03
23	−5631.258605	−5631.248437	−6.38	24	−5669.327994	−5669.329546	0.97
25	−5707.410468	−5707.401326	−5.74				
				6[a]	−4984.560592	−4984.564179	2.25
				6[b]	−6911.628214	−6911.632814	2.89
				6[c]	−4983.951713	−4983.957374	3.55
				6[d]	−4985.134213	−4985.136439	1.40
				6[e]	−4984.561597	−4984.564182	1.62
				6[f]	−227.7959684	−227.8041223	5.12
				6[g]	−228.2275382	−228.2544891	16.91
				6[h]	−228.2804214	−228.3077383	17.14
				6[i]	−228.0689499	−228.0929651	15.07
				6[j]	−228.1353664	−228.1586402	14.60
				6[k]	−228.3170708	−228.3383461	13.35

[a] Electronic energies of $[FeC_6Fe]^{2+}$ with methyl (in dppe) and Cp ligands derived at M06L/DZP level of theory;

[b] Electronic energies of $[FeC_6Fe]^{2+}$ with phenyl (in dppe) and Cp* ligands derived at M06L/DZP level of theory;

[c] Electronic energies of $[FeC_6Fe]^{2+}$ with methyl (in dppe) and Cp ligands derived at M06/TZVP level of theory.

[d] Electronic energies of $[FeC_6Fe]^{2+}$ with methyl (in dppe) and Cp ligands derived at B3LYP/TZVP level of theory.

[e] Electronic energies of $[FeC_6Fe]^{2+}$ with methyl (in dppe) and Cp ligands derived at M06L/DZP level of theory; the singlet state is a antiferromagnetic state roughly optimized.

[f] Electronic energies of uncapped C_6 derived at CCSD(T)/cc-pVTZ level of theory.

[g] Electronic energies of uncapped C_6 derived at M06L/DZP level of theory.

[h] Electronic energies of uncapped C_6 derived at M06L/cc-pVTZ level of theory.

[i] Electronic energies of uncapped C_6 derived at M06/DZP level of theory.

[j] Electronic energies of uncapped C_6 derived at M06/cc-pVTZ level of theory.

[k] Electronic energies of uncapped C_6 derived at B3LYP/cc-pVTZ level of theory.

Table S2. Relative energies, S^2 and number of unpaired electrons (Head-Gordon Index) using spin-flip DFT (SF-DFT) method (non-collinear SF-DFT with PBE0/6-31+G*).

	E_ex, eV	$<S^2>$	$n_{u,nl}$	State
C1	0.00	0.35	0.12	singlet
	0.90	2.50	2.10	triplet
	1.10	1.37	2.10	open-shell singlet (spin-contaminated)
C2	0.00	2.29	2.02	triplet
	0.02	0.19	0.02	singlet
	0.46	0.22	2.02	open-shell singlet
C3	0.00	0.55	0.30	singlet
	0.57	1.69	2.19	triplet
	1.11	1.30	2.52	open-shell singlet (spin-contaminated)
C5	0.00	0.63	0.39	singlet
	0.39	1.63	2.26	triplet
	0.95	1.32	2.51	open-shell singlet (spin-contaminated)
C6	0.00	0.31	0.09	singlet
	0.03	2.23	2.04	triplet
	0.36	0.48	2.06	open-shell singlet

Table S3. Bond distances (Å) of $[FeC_nFe]^{2+}$ chains from one end to another for iron-capped linear carbon dications in singlet and triplet states. Fe−C bond shown in red.

FeC_1Fe		FeC_2Fe		FeC_3Fe		FeC_4Fe		FeC_5Fe	
S	T	S	T	S	T	S	T	S	T
1.734 1.734	1.777 1.777	1.796 1.292 1.796	1.791 1.292 1.791	1.735 1.298 1.298 1.735	1.811 1.304 1.304 1.811	1.781 1.282 1.316 1.282 1.781	1.789 1.278 1.320 1.278 1.789	1.741 1.292 1.290 1.290 1.292 1.741	1.801 1.287 1.300 1.300 1.287 1.801
FeC_6Fe		FeC_7Fe		FeC_8Fe		FeC_9Fe		$FeC_{10}Fe$	
S	T	S	T	S	T	S	T	S	T
1.772 1.283 1.306 1.272 1.306 1.283 1.772	1.768 1.283 1.304 1.274 1.304 1.283 1.768	1.744 1.290 1.292 1.283 1.283 1.292 1.290 1.744	1.792 1.283 1.303 1.284 1.284 1.303 1.283 1.792	1.768 1.283 1.303 1.273 1.297 1.273 1.303 1.283 1.768	1.765 1.284 1.302 1.275 1.295 1.275 1.302 1.284 1.765	1.747 1.289 1.293 1.281 1.284 1.284 1.281 1.293 1.289 1.747	1.787 1.281 1.304 1.279 1.289 1.289 1.279 1.304 1.281 1.787	1.767 1.283 1.302 1.274 1.295 1.274 1.295 1.274 1.302 1.283 1.767	1.764 1.284 1.301 1.275 1.293 1.276 1.293 1.275 1.301 1.284 1.764
$FeC_{11}Fe$		$FeC_{12}Fe$		$FeC_{13}Fe$		$FeC_{14}Fe$		$FeC_{15}Fe$	
S	T	S	T	S	T	S	T	S	T
1.750 1.287 1.294 1.280 1.285 1.282 1.282 1.285 1.280 1.294 1.287 1.750	1.784 1.280 1.305 1.276 1.291 1.283 1.283 1.291 1.276 1.305 1.280 1.784	1.766 1.283 1.302 1.274 1.294 1.275 1.293 1.275 1.294 1.274 1.302 1.283 1.766	1.763 1.284 1.300 1.275 1.292 1.276 1.291 1.276 1.292 1.275 1.300 1.284 1.763	1.753 1.286 1.296 1.278 1.287 1.281 1.283 1.283 1.281 1.287 1.278 1.296 1.286 1.753	1.781 1.280 1.305 1.274 1.293 1.280 1.286 1.286 1.280 1.293 1.274 1.305 1.280 1.781	1.766 1.282 1.302 1.274 1.293 1.275 1.292 1.275 1.292 1.275 1.293 1.274 1.302 1.282 1.766	1.764 1.283 1.300 1.275 1.292 1.277 1.290 1.277 1.290 1.277 1.292 1.275 1.300 1.283 1.764	1.755 1.285 1.297 1.277 1.288 1.280 1.285 1.282 1.282 1.285 1.280 1.288 1.277 1.297 1.285 1.755	1.779 1.280 1.305 1.273 1.294 1.278 1.288 1.283 1.283 1.288 1.278 1.293 1.273 1.305 1.280 1.779

$FeC_{16}Fe$		$FeC_{17}Fe$		$FeC_{18}Fe$		$FeC_{19}Fe$		$FeC_{20}Fe$	
S	T	S	T	S	T	S	T	S	T
1.767	1.765	1.757	1.778	1.768	1.766	1.760	1.778	1.769	1.767
1.282	1.283	1.284	1.279	1.281	1.282	1.283	1.279	1.281	1.282
1.302	1.301	1.298	1.305	1.302	1.301	1.299	1.305	1.303	1.302
1.274	1.275	1.276	1.273	1.273	1.274	1.276	1.272	1.273	1.274
1.293	1.292	1.289	1.294	1.293	1.292	1.290	1.295	1.294	1.292
1.275	1.277	1.279	1.277	1.275	1.276	1.278	1.276	1.275	1.276
1.291	1.290	1.286	1.289	1.291	1.289	1.287	1.290	1.291	1.290
1.276	1.277	1.281	1.281	1.276	1.277	1.280	1.279	1.276	1.277
1.291	1.289	1.283	1.285	1.290	1.288	1.284	1.286	1.290	1.288
1.276	1.277	1.283	1.285	1.276	1.278	1.282	1.283	1.277	1.278
1.291	1.290	1.281	1.281	1.290	1.288	1.282	1.283	1.289	1.288
1.275	1.277	1.286	1.289	1.276	1.277	1.284	1.286	1.277	1.278
1.293	1.292	1.279	1.277	1.291	1.289	1.280	1.279	1.290	1.288
1.274	1.275	1.289	1.294	1.275	1.276	1.287	1.290	1.276	1.277
1.302	1.301	1.276	1.273	1.293	1.292	1.278	1.276	1.291	1.290
1.282	1.283	1.298	1.305	1.273	1.274	1.290	1.295	1.275	1.276
1.767	1.765	1.284	1.279	1.302	1.301	1.276	1.272	1.294	1.292
		1.757	1.778	1.281	1.282	1.299	1.305	1.303	1.302
				1.768	1.766	1.283	1.279	1.281	1.282
						1.760	1.778	1.769	1.767

$FeC_{21}Fe$		$FeC_{22}Fe$		$FeC_{23}Fe$		$FeC_{24}Fe$		$FeC_{25}Fe$	
S	T	S	T	S	T	S	T	S	T
1.761	1.778	1.770	1.768	1.763	1.777	1.770	1.769	1.765	1.778
1.283	1.279	1.281	1.281	1.282	1.279	1.280	1.281	1.281	1.278
1.300	1.305	1.303	1.302	1.300	1.306	1.303	1.303	1.301	1.306
1.275	1.272	1.273	1.274	1.274	1.272	1.272	1.273	1.274	1.271
1.291	1.295	1.294	1.293	1.291	1.295	1.294	1.293	1.292	1.296
1.277	1.275	1.274	1.276	1.276	1.274	1.274	1.275	1.276	1.274
1.288	1.291	1.291	1.290	1.288	1.291	1.292	1.290	1.289	1.292
1.279	1.278	1.276	1.277	1.278	1.277	1.275	1.277	1.278	1.276
1.285	1.287	1.290	1.288	1.286	1.288	1.290	1.289	1.287	1.289
1.281	1.281	1.276	1.278	1.280	1.280	1.276	1.278	1.280	1.279
1.283	1.284	1.289	1.287	1.284	1.285	1.289	1.287	1.285	1.286
1.283	1.284	1.277	1.279	1.282	1.283	1.277	1.279	1.281	1.282
1.281	1.281	1.289	1.287	1.282	1.283	1.289	1.287	1.283	1.284
1.285	1.287	1.276	1.278	1.284	1.285	1.277	1.279	1.283	1.284
1.279	1.278	1.290	1.288	1.280	1.280	1.289	1.287	1.281	1.282
1.288	1.291	1.276	1.277	1.286	1.288	1.276	1.278	1.285	1.286

1.277	1.275	1.291	1.290	1.278	1.277	1.290	1.289	1.280	1.279
1.291	1.295	1.274	1.276	1.288	1.291	1.275	1.277	1.287	1.289
1.275	1.272	1.294	1.293	1.276	1.274	1.292	1.290	1.278	1.276
1.300	1.305	1.273	1.274	1.291	1.295	1.274	1.275	1.289	1.292
1.283	1.279	1.303	1.302	1.274	1.272	1.294	1.293	1.276	1.274
1.761	1.778	1.281	1.281	1.300	1.306	1.272	1.273	1.292	1.296
		1.770	1.768	1.282	1.279	1.303	1.303	1.274	1.271
				1.763	1.777	1.280	1.281	1.301	1.306
						1.770	1.769	1.281	1.278
								1.765	1.778

Table S4. Mayer bond order between adjacent atoms in the chain from one end to another for iron-capped linear carbon dications $[FeC_nFe]^{2+}$ in singlet and triplet states; Fe-C bond orders shown in red. *averages C−C MBOs and MBO ranges.

C=C(allene)		1.880, 1.880				C=C(ethylene)		1.912	
C≡C(acetylene)		2.875				C−C(ethane)		0.936	
FeC_1Fe		FeC_2Fe		FeC_3Fe		FeC_4Fe		FeC_5Fe	
S	T	S	T	S	T	S	T	S	T
1.325 1.325	1.212 1.212	1.259 1.766 1.259	1.144 1.703 1.144	1.259 1.615 1.615 1.259	1.057 1.546 1.546 1.057	1.225 1.505 2.028 1.504 1.225	1.137 1.518 1.972 1.518 1.137	1.354 1.681 1.764 1.764 1.681 1.354	1.135 1.728 1.694 1.694 1.728 1.135
		1.766* □0.000	1.703 □0.000	1.615 □0.000	1.546 □0.000	1.679 □0.262	1.669 □0.227	1.723 □0.042	1.711 □0.017
FeC_6Fe		FeC_7Fe		FeC_8Fe		FeC_9Fe		$FeC_{10}Fe$	
S	T	S	T	S	T	S	T	S	T
1.248 1.723 1.843 1.632 1.843 1.723 1.248	1.199 1.689 1.835 1.603 1.835 1.689 1.199	1.316 1.604 1.986 1.660 1.660 1.986 1.604 1.316	1.150 1.679 1.878 1.679 1.679 1.878 1.679 1.150	1.261 1.724 1.843 1.783 1.791 1.783 1.843 1.724 1.261	1.221 1.693 1.834 1.751 1.806 1.751 1.834 1.693 1.221	1.294 1.632 1.954 1.634 1.866 1.866 1.634 1.954 1.632 1.294	1.161 1.702 1.859 1.678 1.83 1.83 1.679 1.86 1.702 1.162	1.262 1.697 1.882 1.758 1.731 1.978 1.731 1.758 1.882 1.698 1.261	1.229 1.676 1.877 1.736 1.739 1.95 1.738 1.736 1.877 1.676 1.229
1.753 □0.106	1.730 □0.116	1.750 □0.191	1.745 □0.099	1.784 □0.060	1.766 □0.071	1.772 □0.161	1.768 □0.091	1.791 □0.141	1.778 □0.137
$FeC_{11}Fe$		$FeC_{12}Fe$		$FeC_{13}Fe$		$FeC_{14}Fe$		$FeC_{15}Fe$	
S	T	S	T	S	T	S	T	S	T
1.279	1.171	1.253	1.223	1.27	1.183	1.246	1.222	1.258	1.186
1.658	1.721	1.692	1.672	1.665	1.721	1.697	1.68	1.67	1.721
1.920	1.837	1.895	1.889	1.912	1.843	1.888	1.885	1.911	1.85
1.674	1.723	1.73	1.709	1.693	1.741	1.728	1.71	1.696	1.743
1.854	1.807	1.761	1.771	1.817	1.77	1.779	1.788	1.804	1.759
1.831	1.826	1.959	1.935	1.874	1.883	1.929	1.908	1.897	1.912
1.831	1.827	1.689	1.695	1.810	1.792	1.724	1.732	1.773	1.749
1.854	1.807	1.959	1.936	1.810	1.792	1.943	1.922	1.852	1.847
1.674	1.723	1.761	1.77	1.874	1.883	1.724	1.732	1.852	1.846

1.920 1.658 1.279	1.838 1.719 1.172	1.730 1.895 1.692 1.253	1.71 1.89 1.672 1.225	1.817 1.693 1.912 1.665 1.270	1.77 1.741 1.843 1.721 1.183	1.929 1.779 1.728 1.888 1.697 1.246	1.908 1.787 1.71 1.885 1.681 1.221	1.773 1.897 1.804 1.696 1.911 1.67 1.258	1.75 1.911 1.76 1.742 1.851 1.721 1.185
1.787 □0.131	1.783 □0.060	1.797 □0.135	1.786 □0.132	1.795 □0.124	1.792 □0.081	1.803 □0.123	1.794 □0.121	1.800 □0.121	1.797 □0.095
$FeC_{16}Fe$		$FeC_{17}Fe$		$FeC_{18}Fe$		$FeC_{19}Fe$		$FeC_{20}Fe$	
S	T	S	T	S	T	S	T	S	T
1.239 1.703 1.883 1.734 1.775 1.927 1.739 1.912 1.761 1.912 1.739 1.927 1.775 1.734 1.883 1.703 1.239	1.217 1.688 1.881 1.717 1.783 1.907 1.747 1.892 1.77 1.892 1.747 1.907 1.783 1.717 1.881 1.688 1.217	1.248 1.677 1.906 1.700 1.801 1.900 1.762 1.876 1.815 1.815 1.876 1.762 1.900 1.801 1.700 1.906 1.677 1.248	1.189 1.719 1.853 1.742 1.761 1.918 1.737 1.878 1.803 1.803 1.878 1.737 1.919 1.76 1.742 1.854 1.72 1.189	1.234 1.705 1.882 1.735 1.770 1.934 1.734 1.908 1.776 1.880 1.776 1.908 1.734 1.934 1.770 1.735 1.882 1.705 1.234	1.214 1.692 1.88 1.72 1.778 1.915 1.743 1.89 1.787 1.861 1.787 1.89 1.743 1.915 1.778 1.72 1.88 1.692 1.214	1.239 1.684 1.899 1.706 1.796 1.904 1.760 1.880 1.804 1.839 1.839 1.804 1.880 1.760 1.904 1.796 1.706 1.899 1.684 1.239	1.189 1.722 1.855 1.745 1.758 1.924 1.735 1.886 1.79 1.834 1.834 1.79 1.886 1.735 1.924 1.758 1.745 1.855 1.722 1.189	1.228 1.707 1.882 1.735 1.768 1.937 1.729 1.915 1.772 1.876 1.794 1.876 1.772 1.915 1.729 1.937 1.768 1.735 1.882 1.707 1.228	1.209 1.695 1.88 1.721 1.776 1.919 1.737 1.897 1.783 1.857 1.805 1.857 1.783 1.897 1.737 1.919 1.776 1.721 1.88 1.695 1.209
1.807 □0.112	1.800 □0.110	1.805 □0.115	1.802 □0.100	1.810 □0.115	1.804 □0.112	1.808 □0.110	1.805 □0.101	1.812 □0.115	1.807 □0.112
$FeC_{21}Fe$		$FeC_{22}Fe$		$FeC_{23}Fe$		$FeC_{24}Fe$		$FeC_{25}Fe$	
S	T	S	T	S	T	S	T	S	T
1.231 1.69 1.895 1.712 1.789	1.189 1.723 1.856 1.747 1.755	1.222 1.71 1.880 1.737 1.766	1.204 1.698 1.879 1.723 1.773	1.223 1.695 1.891 1.716 1.783	1.188 1.724 1.857 1.748 1.753	1.216 1.713 1.878 1.739 1.763	1.2 1.703 1.877 1.726 1.77	1.217 1.7 1.888 1.72 1.778	1.186 1.726 1.857 1.749 1.751

1.911	1.931	1.938	1.923	1.918	1.936	1.941	1.926	1.924	1.941
1.754	1.73	1.727	1.735	1.747	1.725	1.725	1.733	1.741	1.72
1.883	1.893	1.917	1.9	1.89	1.901	1.919	1.902	1.897	1.908
1.803	1.786	1.768	1.778	1.797	1.78	1.766	1.777	1.79	1.774
1.842	1.842	1.881	1.863	1.845	1.849	1.883	1.865	1.852	1.857
1.828	1.82	1.790	1.802	1.826	1.815	1.786	1.799	1.821	1.809
1.828	1.82	1.871	1.852	1.831	1.827	1.876	1.857	1.834	1.834
1.842	1.842	1.790	1.802	1.831	1.827	1.787	1.8	1.829	1.823
1.803	1.786	1.881	1.863	1.826	1.815	1.876	1.857	1.829	1.823
1.883	1.893	1.768	1.778	1.845	1.849	1.786	1.799	1.834	1.834
1.754	1.73	1.917	1.9	1.797	1.78	1.883	1.865	1.821	1.809
1.911	1.931	1.727	1.735	1.89	1.901	1.766	1.777	1.852	1.857
1.789	1.755	1.938	1.923	1.747	1.725	1.919	1.902	1.790	1.774
1.712	1.747	1.766	1.773	1.918	1.936	1.725	1.733	1.897	1.908
1.895	1.856	1.737	1.723	1.783	1.753	1.941	1.926	1.741	1.72
1.690	1.723	1.88	1.879	1.716	1.748	1.763	1.77	1.924	1.941
1.231	1.189	1.71	1.698	1.891	1.857	1.739	1.726	1.778	1.751
		1.222	1.205	1.695	1.724	1.878	1.877	1.720	1.75
				1.223	1.187	1.713	1.704	1.888	1.857
						1.216	1.2	1.700	1.726
								1.217	1.186
1.811	1.808	1.814	1.810	1.813	1.810	1.816	1.812	1.815	1.812
□0.111	□0.104	□0.114	□0.113	□0.112	□0.106	□0.114	□0.112	□0.112	□0.111