

Electronic Supplementary Information

Intrinsically conducting polyaminoanthraquinone nanofibrils: Interfacial synthesis, formation mechanism and lead adsorbents

Shao-Jun Huang,^{*a} Chun-Gang Min,^a Yaozu Liao,^{*b,d} Ping Du,^a Hui Sun,^a Yan-Qin Zhu^a and Ai-Min Ren^c

^a Research Center for Analysis and Measurement, Kunming University of Science and Technology, Kunming, 650093, China. Fax: +86-871-65111617; Tel: +86-871-65113971; E-mail: huangshaojun1975@163.com

^b School of Chemistry, University of Bristol, Bristol, England BS8 1TS, UK. E-mail: yaozu.liao@gmail.com

^c State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry, Jilin University, Changchun, 130023, China

^d School of Materials Science and Engineering, University of Shanghai for Science and Technology, Shanghai, 200092, China

Table S1 Main atomic electron density populations for ACA

Atom	Electric charge	Atom	Electric charge
C(2)	-0.26599	C(8)	-0.19096
C(3)	-0.19184	N(1)	-0.79399
C(4)	-0.22077	O(9)	-0.59980
C(6)	-0.22813	O(10)	-0.52374
C(7)	-0.20445	Cl(5)	0.04223

Table S2 Main composition and proportion of frontier orbitals in ACA (%)

Atom	HOMO-1	HOMO	LUMO	LUMO+1
C(2)	0.1	12.6	5.6	0.9
C(3)	0.3	0.5	4.1	3.4
C(4)	2.5	18.5	3.7	4.6
C(6)	0.9	0.4	4.0	6.7
C(7)	0.2	0.0	4.8	5.6
C(8)	1.4	0.4	1.5	18.0
N(1)	0.5	36.5	1.9	3.5
O(9)	5.0	4.0	13.9	4.6
O(10)	40.9	2.6	15.4	5.4
Cl(5)	12.5	0.1	0.7	3.1

Table S3 Main atomic electron spin densities for ACA

Atom	Electron spin density	Atom	Electron spin density
C(2)	0.221341	C(8)	0.025446
C(3)	-0.127492	N(1)	0.408262
C(4)	0.345231	O(9)	0.014812
C(6)	0.030662	O(10)	0.006762
C(7)	-0.012947	Cl(5)	0.014604

Table S4 Main atomic electron density populations for PACA molecule with 10 repeating units

Atom	Electric charge	Atom	Electric charge	Atom	Electric charge	Atom	Electric charge	Atom	Electric charge	Atom	Electric charge
C 1	-0.08981	C 42	-0.18812	C 83	0.24365	O 124	-0.55597	C 165	-0.14971	H 206	0.25766
C 2	-0.1226	C 43	0.53067	C 84	-0.24829	Cl 125	0.03925	C 166	-0.09513	H 207	0.2482
C 3	-0.00855	C 44	-0.14444	C 85	-0.20805	N 126	-0.57923	C 167	-0.20245	H 208	0.26595
C 4	-0.22971	C 45	-0.10907	C 86	0.16566	N 127	-0.58183	C 168	-0.19933	H 209	0.24729
C 5	-0.20856	C 46	0.54114	O 87	-0.53283	C 128	0.21493	C 169	-0.24904	H 210	0.24987
C 6	-0.19134	C 47	0.2132	O 88	-0.59264	C 129	-0.14383	C 170	0.53197	H 211	0.46021
C 7	0.52461	C 48	-0.24382	Cl 89	0.03822	C 130	-0.11197	C 171	-0.09593	H 212	0.48147
C 8	-0.17487	C 49	-0.21582	N 90	-0.61196	C 131	0.17196	C 172	-0.13543	H 213	0.24778
C 9	-0.11759	C 50	0.16832	N 91	-0.58351	C 132	-0.22378	C 173	0.55157	H 214	0.24975
C 10	0.53224	O 51	-0.53076	C 92	0.21144	C 133	-0.24759	C 174	-0.18624	H 215	0.26687
C 11	0.23281	O 52	-0.55788	C 93	-0.14383	C 134	0.53019	C 175	-0.19747	H 216	0.24823
C 12	-0.2415	Cl 53	0.03793	C 94	-0.1223	C 135	-0.09267	C 176	-0.22239	H 217	0.25738
C 13	-0.21929	N 54	-0.57814	C 95	0.18316	C 136	-0.12586	C 177	-0.00661	H 218	0.25835
C 14	0.16591	N 55	-0.58691	C 96	-0.23161	C 137	0.53782	O 178	-0.54774	H 219	0.24952
O 15	-0.54332	C 56	0.23071	C 97	-0.23908	C 138	-0.18706	O 179	-0.56887	H 220	0.26803
O 16	-0.60273	C 57	-0.15665	C 98	0.52957	C 139	-0.2044	Cl 180	0.05095	H 221	0.2518
Cl 17	0.03574	C 58	-0.10005	C 99	-0.09194	C 140	-0.22639	H 181	0.25627	H 222	0.25086
N 18	-0.7891	C 59	0.14142	C 100	-0.12303	C 141	-0.00818	H 182	0.24625	H 223	0.48165
N 19	-0.58041	C 60	-0.19731	C 101	0.53415	O 142	-0.5334	H 183	0.26451	H 224	0.48228
C 20	0.20653	C 61	-0.25754	C 102	-0.18853	O 143	-0.56006	H 184	0.24457	H 225	0.25231
C 21	-0.14355	C 62	0.53126	C 103	-0.20654	Cl 144	0.03874	H 185	0.24754	H 226	0.252
C 22	-0.1251	C 63	-0.09107	C 104	-0.22815	C 145	-0.08831	H 186	0.42732	H 227	0.26826
C 23	0.19016	C 64	-0.12829	C 105	-0.00859	C 146	-0.12835	H 187	0.44334	H 228	0.24975
C 24	-0.23034	C 65	0.54499	O 106	-0.53866	C 147	-0.00622	H 188	0.48205	H 229	0.25853
C 25	-0.23696	C 66	-0.18904	O 107	-0.56528	C 148	-0.22623	H 189	0.25156	H 230	0.26034
C 26	0.5276	C 67	-0.20597	Cl 108	0.03674	C 149	-0.19996	H 190	0.253	H 231	0.25085
C 27	-0.09228	C 68	-0.22794	C 109	-0.09288	C 150	-0.1854	H 191	0.26645	H 232	0.27068
C 28	-0.1226	C 69	-0.01085	C 110	-0.12529	C 151	0.52406	H 192	0.24739	H 233	0.25339
C 29	0.53271	O 70	-0.51049	C 111	-0.0084	C 152	-0.14475	H 193	0.2567	H 234	0.25299
C 30	-0.18988	O 71	-0.56247	C 112	-0.22661	C 153	-0.128	H 194	0.25777	H 235	0.48315
C 31	-0.20796	Cl 72	0.03834	C 113	-0.20474	C 154	0.53987	H 195	0.24873	H 236	0.47674
C 32	-0.22945	C 73	-0.09197	C 114	-0.18721	C 155	0.21602	H 196	0.26781	H 237	0.26177
C 33	-0.00904	C 74	-0.12126	C 115	0.53074	C 156	-0.2355	H 197	0.26381	H 238	0.24778
O 34	-0.53997	C 75	-0.00882	C 116	-0.13862	C 157	-0.2314	H 198	0.26596	H 239	0.25282
O 35	-0.56707	C 76	-0.22597	C 117	-0.116	C 158	0.19527	H 199	0.48114	H 240	0.26986
Cl 36	0.03695	C 77	-0.20732	C 118	0.53773	O 159	-0.58788	H 200	0.47849	H 241	0.25354
C 37	-0.09178	C 78	-0.18747	C 119	0.20857	O 160	-0.56873	H 201	0.25026	H 242	0.2628
C 38	-0.12623	C 79	0.5365	C 120	-0.24424	Cl 161	0.04007	H 202	0.25111		
C 39	-0.00847	C 80	-0.14686	C 121	-0.22867	N 162	-0.57783	H 203	0.26693		
C 40	-0.22741	C 81	-0.10676	C 122	0.17886	N 163	-0.57716	H 204	0.24866		
C 41	-0.20531	C 82	0.5372	O 123	-0.53386	C 164	0.21327	H 205	0.25779		

Table S5 Solubility and solution color of ACA monomer and PACA prepared with an initial ACA concentration of 142.9 mmol/L and a CrO₃/ACA molar ratio of 2.0 in a 250 mmol/L of HClO₄ biphasic system of C₆H₅NO₂/H₂O (6:1, v/v) at 20 °C for 72 h.

	Solubility ^a and solution color ^b						
	THF	DMF	NMP	DMSO	Water	0.5 M HCl	0.5 M NaOH
PACA polymer	WS (lc)	PS (dc)	PS (dc)	PS (dc)	IS	IS	IS
ACA monomer	S (or)	S (rb)	S (rb)	S (rb)	IS	IS	IS

^a Solubility: IS–insoluble, WS–weakly soluble, PS–partially soluble, S–soluble; ^b Solution color: rb–reddish brown, or–orange red, dc–dark cyan, lc–light cyan.

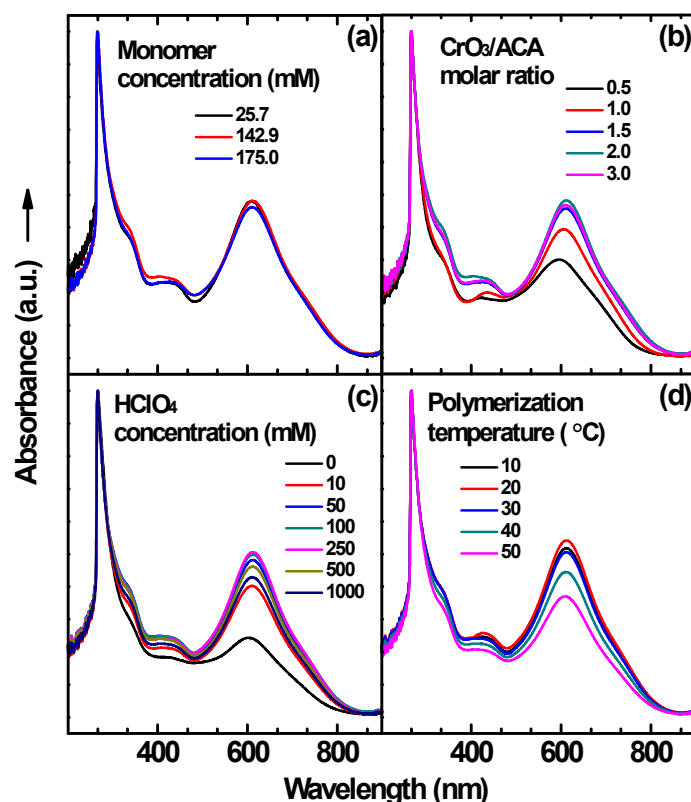


Fig. S1 Normalized UV–vis absorption spectra of PACAs prepared with (a) different initial ACA concentrations and a CrO₃/ACA molar ratio of 2.0 in a 50 mmol/L HClO₄ biphasic system of C₆H₅NO₂/H₂O (6:1, v/v) at 30 °C for 72 h; (b) an initial ACA concentration of 142.9 mmol/L and different CrO₃/ACA molar ratios in a 50 mmol/L HClO₄ biphasic system of C₆H₅NO₂/H₂O (6:1, v/v) at 30 °C for 72 h; (c) an initial ACA concentration of 142.9 mmol/L and a CrO₃/ACA molar ratio of 2.0 in a biphasic system of C₆H₅NO₂/H₂O (6:1, v/v) containing different concentrations of HClO₄ at 30 °C for 72 h; and (d) an initial ACA concentration of 142.9 mmol/L and a CrO₃/ACA molar ratio of 2.0 in a 250 mmol/L HClO₄ biphasic system of C₆H₅NO₂/H₂O (6:1, v/v) at different temperatures for 72 h. DMF was used as solvent for UV-vis spectral tests.

Fig. S2 Dispersions of the PACA nanofibrils upon adding NaCl electrolyte after standing for 24 h.

Fig. S3 Pictures of ACA powders, PACA powders and resultant coke made from PACA.