Supplementary Information For:

Boron-Doped Coronenes with High Redox Potential for Organic Positive Electrodes in Lithium-Ion Batteries: First-Principles Density Functional Theory Modeling Study

Yuntong Zhu,[a] Ki Chul Kim*[b] and Seung Soon Jang*[acd]

[a]Computational NanoBio Technology Laboratory, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332-0245, USA
[b]Department of Chemical Engineering, Konkuk University, Seoul 05029, Republic of Korea
[c]Institute for Electronics and Nanotechnology, Georgia Institute of Technology, Atlanta, GA 30332, USA
[d]Parker H. Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, GA 30332, USA

Corresponding Authors:

kich2018@konkuk.ac.kr; seungsoon.jang@mse.gatech.edu

Table S1. The most stable spin multiplicities for the pristine coronene and its boron-doped derivatives at the neutral and anionic charge states

Structure		The most stable spin multiplicity	
Dopant(s)	**Case**	**Neutral**	**Anion**
0	P	1	2
1	B1-1	2	1
	B1-2	2	1
	B1-3	2	1
2	B2-1	1	2
	B2-2	1	2
	B2-3	1	2
	B2-4	3	2
	B2-5	1	2
	B2-6	1	4
	B2-7	1	2
	B2-8	1	2
	B2-9	1	2
	B2-10	1	2
	B2-11	1	2
	B2-12	1	2
	B2-13	3	2

	B2-14	1	2
	B2-15	1	2
	B2-16	1	2
	B2-17	1	2
	B2-18	1	2
	B2-19	1	2
	B2-20	1	2
	B2-21	1	2
	B2-22	1	2
	B2-23	1	2
	B2-24	1	2
	B2-25	1	2
	B2-26	3	2
	B2-27	1	2
	B2-28	3	2
	B2-29	1	2
	B2-30	1	2
	B2-31	1	2

Table S2. Redox potentials of pristine coronene and its boron-doped derivatives in vacuum and solution (corresponding to the mixture of ethylene carbonate and dimethyl carbonate with the molar ratio of 3:7). The contribution of the solvation to the redox potential is calculated by the difference in the redox potential between vacuum and solution phases.

Structure		Redox potential (V vs. Li/Li^+)		Solvation contribution (V)
Doopant (s)	Case	In vacuum	In solution	
0	P	-0.91	0.67	1.58
1	B1-1	3.78	5.42	1.64
	B1-2	3.69	5.30	1.61
	B1-3	3.64	5.28	1.64
2	B2-1	0.90	2.61	1.71
	B2-2	1.29	2.92	1.63
	B2-3	1.99	3.57	1.58
	B2-4	1.46	3.06	1.60
	B2-5	-2.05	-0.39	1.66
	B2-6	-1.14	0.42	1.56
	B2-7	-1.17	0.46	1.63
	B2-8	-1.22	0.38	1.60
	B2-9	-0.03	1.45	1.48
	B2-10	1.36	3.00	1.64
	B2-11	1.74	3.28	1.54
	B2-12	1.39	2.95	1.56
	B2-12	1.51	3.07	1.56

	B2-14	1.19	2.79	1.60
	B2-15	1.52	3.13	1.61
	B2-16	-1.19	0.50	1.69
	B2-17	0.18	1.82	1.64
	B2-18	-1.22	0.40	1.62
	B2-19	0.23	1.93	1.70
	B2-20	1.72	3.33	1.61
	B2-21	1.48	3.10	1.62
	B2-22	-0.50	1.12	1.62
	B2-23	2.12	3.81	1.69
	B2-24	2.69	4.35	1.66
	B2-25	-0.31	1.37	1.68
	B2-26	1.47	3.13	1.66
	B2-27	1.54	3.16	1.62
	B2-28	1.54	3.14	1.60
	B2-29	1.60	3.18	1.58
	B2-30	1.66	3.25	1.59
	B2-31	1.06	2.70	1.64

Table S3. Local (or atomic) spin states for the B2-3 case in gas phase.

Atom	C1	C2	C3	C4	C5	C6
Spin state	-0.00098	0.00042	-0.00181	0.00260	-0.00021	0.00221
Atom	C7	C8	C9	C10	C11	C12
Spin state	0.00475	-0.00133	0.00062	-0.00027	-0.00141	0.00284
Atom	C13	C14	C15	C16	C17	C18
Spin state	-0.00100	0.00213	0.00121	-0.00127	0.00166	0.00147
Atom	C19	B20	C21	C22	C23	B24
Spin state	-0.00132	0.00046	-0.00793	0.00055	-0.00372	0.00019
Atom	H25	H26	H27	H28	H29	H30
Spin state	-0.00005	-0.00003	-0.00012	0.00002	-0.00002	0.00004
Atom	H31	H32	H33	H34	H35	H36
Spin state	-0.00006	0.00005	0.00001	0.00026	0.00006	-0.00003

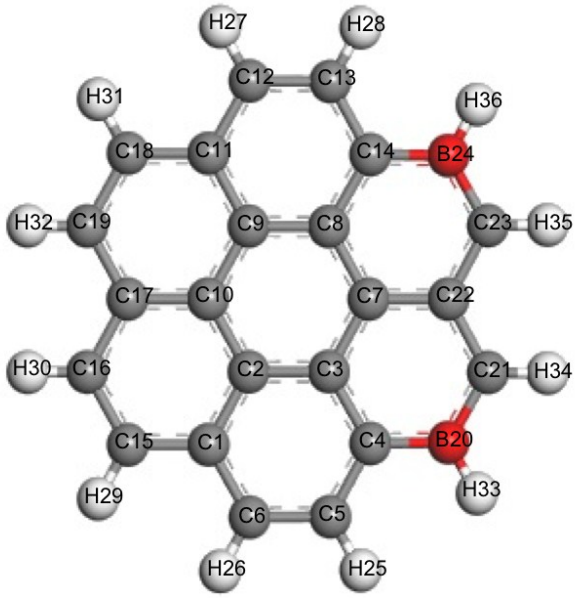

Figure S1. The structure of B2-3 with labelled atom numbers.