## Structure-electrochemical property relationship of quinone electrodes for lithium-ion batteries<sup>†</sup>

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**Table S1.** The geometries of lithiated, sodiated, and potassiated 20 quinone isomers. The BE (in kcal/mol), and redox potentials (in V) of them. The atoms in gray, white, red, lilac, violet, and modena denote those of carbon, hydrogen, oxygen, lithium, sodium, and potassium, respectively.

	Li		N	Na		К	
	case 1	case 2	case 1	case 2	case 1	case 2	
	्र ३- <b>०</b> -३ ३-२,	3-3 3-3 3-3 3-3 3-3 3-3 3-3 3-3 3-3 3-3	3-3 9-3 9-3 3-3 3-3	9-0 9-0 9-0 9-0	9-9-9 9-9-9 9-9-9	9-0 9-0 9-0 9-0	
1 4-BO	BE1=-68.6	BE2=-65.3	BE1 <b>=-49.6</b>	BE2=-37.1	BE1=- <b>55.5</b>	BE2 <b>=-40.1</b>	
1, <b>4-DQ</b>	E1 <b>=2.66</b>	E <sub>2</sub> =2.45	E1=1.88	E <sub>2</sub> =1.35	E1 <b>=2.17</b>	E2=1.38	
LUMO3.733	E=2	2.55	E=	1.61	E=	1.77	
	موجوع بالارجام	؞؞ ؞ ؞ڡۛ؞ۣڡؘ	موني من من من من من من من من من م	م مينفي رغيفي	مي هرمه باهي هي باهي هي	موند می موند با	
	BE1 <b>=-93.8</b>	BE2 <b>=-66.9</b>	BE1 <b>=-71.4</b>	BE2 <b>=-45.7</b>	BE1 <b>=-73.3</b>	BE2 <b>=-48.7</b>	
1,2-BQ	E1 <b>=3.67</b>	E <sub>2</sub> =2.50	E1 <b>=2.74</b>	E2=1.58	E1 <b>=2.85</b>	E <sub>2</sub> =1.71	
LUMO <b>=-3.829</b>	E=3	3.08	E=	2.16	E=:	2.28	
	ې دوغوغور رغوغوغې	ې د مېښې د مېښې مې د مېښې	ې دونونو رونونو	မှ သူ့ဆို ပူဆို ပူဆို ပ သမိပ္ပေဆီပူဆီပု မ	ې د مېغې کې د مېغې کې	မ သွန်သွန်သွန သိမ္မသူမိသ မ	
	BE1=-62.5	BE2 <b>=-61.8</b>	BE1=-43.5	BE2=-34.3	BE1 <b>=-49.4</b>	BE2 <b>=-38.0</b>	
1,4-NQ	E1 <b>=2.38</b>	E2= <b>2.29</b>	E1 <b>=1.62</b>	E <sub>2</sub> =1.22	E1=1.88	E <sub>2</sub> =1.35	
LUMO <b>=-3.412</b>	E=2	2.33	E=	1.42	E=	1.61	
	ىرىقى قىرى بەرچەرچەر	းမွန်းမှုန်း ၂မီဇွမ်းမွန်း	းမွန် မွန်မှုန် ၂မိမ္မမိမှုမိ ၂မိမ္မမိမှုမိ	ي پونغي≎ پغيغيغي	، يوغي في بغي في في	းမွန်မှုန်မှုန်း အမွန်မွန်း	
	BE1 <b>=-87.6</b>	BE2 <b>=-61.5</b>	BE1 <b>=-65.0</b>	BE2=-41.1	BE1 <b>=-66.8</b>	BE2 <b>=-44.7</b>	
1,2-NQ	E1= <b>3.39</b>	E <sub>2</sub> =2.26	E1 <b>=2.45</b>	E <sub>2</sub> =1.39	E1 <b>=2.55</b>	E <sub>2</sub> =1.55	
LUMO=- <b>3.474</b>	E=2	2.83	E=	1.92	E=:	2.05	

	ؠۑۿۑۿۑ ؠۿۑۿۑۿؠ ؠۿۑۿۑۿؠ	ى قى قى ئەر بولغان قى قى ئەر بەر يەر يەر بەر يەر يەر بەر يەر يەر بەر يەر يەر يەر يەر بەر يەر يەر يەر يەر يەر يەر بەر يەر يەر يەر يەر يەر يەر يەر يەر يەر ي	ې د و و فو فر د فو فر فر	ي قسون دي قي قي قي ي قي قي قر قسي ع	۹ بوغوغی رغوغیفی	ي ميڭرىقى يغرىقى م
1.5-NO	BE1=-76.3	BE2=-72.2	BE1=- <b>56.9</b>	BE2=-50.2	BE1 <b>=-62.6</b>	BE2=-51.2
1,5-11Q	E1= <b>3.00</b>	E <sub>2</sub> =2.74	E1 <b>=2.20</b>	E <sub>2</sub> =1.74	E <sub>1</sub> =2.45	E2 <b>=1.96</b>
LUMO <b>=-4.001</b>	E=2		E=	1.97	E=2	2.20
	دو قوقو و ه دفوقو فر	دو قدو قدو ه رفو قدو قد	دوقو وقو رقو قوقو	دوقو وقر دوقوقو وقر دقوقوقر	دوقو وقو رقو قوقو	د و هې د د و ه و ه و ه د ه و ه و ه ر
	BE1=- <b>77.1</b>	BE2 <b>=-69.7</b>	BE1 <b>=-56.3</b>	BE2 <b>=-47.6</b>	BE1 <b>=-63.3</b>	BE2 <b>=-49.4</b>
1,7-NQ	E1= <b>3.01</b>	E <sub>2</sub> =2.62	E1 <b>=2.16</b>	E <sub>2</sub> =1.68	E1=2.48	E2=1.77
LUMO <b>=-3.945</b>	E=2	2.82	E=	1.92	E=2	2.12
	ي هو مي موجوع موجوع موجوع موجوع	ిల్లె పెంచి పెం పెంచి సెం సెం సెం సెం సెం సెం సెం సెం సెం సెం	تو هو موجوع موجوع موجوع موجوع	يو قوي مان قوي مان قوي مان قوي مان قوي	, <b>, , , , , , , , , , , , , , , , , , </b>	- 30 30 00 - 30 30 00 - 30 30 - 30 30 - 30 30 - 30 30 - 30 30
	BE1=- <b>99.8</b>	BE2=-73.1	BE1=- <b>77.7</b>	BE2=- <b>52.7</b>	BE1=- <b>79.7</b>	BE2 <b>=-56.2</b>
2,3-11Q	E1= <b>3.94</b>	E <sub>2</sub> =2.75	E1 <b>=3.01</b>	E <sub>2</sub> =1.87	E1=3.13	E2= <b>2.03</b>
LUMO <b>=-4.124</b>	E=3	3.34	E=	2.44	E=2	2.58
0	းမွန်မွန်မွန <sup>က</sup> စင်မွန်မွန်း	؞ۑۿٚۑۿٚۑ؋ ۑڡۿڮۣۿڮۿ	-يۇغىغە <sup>-ئە</sup> مەيغىغە	، يەرەپەرە رەپەيە	-يقيقي• <sup>-0</sup> •قيقية,	مىقىقى. رەيغىقى
2.6-NO	BE1=-73.3	BE2 <b>=-70.6</b>	BE1 <b>=-54.0</b>	BE <sub>2</sub> =-44.6	BE1 <b>=-59.9</b>	BE2 <b>=-48.1</b>
LUMO=-3.881	E1 <b>=2.86</b>	E <sub>2</sub> =2.66	E1 <b>=2.08</b>	E <sub>2</sub> =1.62	E1 <b>=2.33</b>	E2=1.76
	E=2	2.76	E=	1.85	E=2	2.05
	မှ နိုင်ငံနှင့် မိုင်ငံ ကို မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မို ကို မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင်ငံနှင့် မိုင		မှ းဆိုမှုဆိုမှုဆို ဖြစ်မှုဆိုမှုဆို	ين ياقي يويغي غريقي يغي غريقي وي	ې د پېڅې څې څې د اغ پېڅې څې د	
	BE1=-70.6	BE2= <b>-65.0</b>	BE1 <b>=-51.1</b>	BE2= <b>-44.8</b>	BE1 <b>=-56.7</b>	BE2= <b>-48.1</b>
1,10-AQ	E1=2.73	E <sub>2</sub> =2.45	E1 <b>=1.94</b>	E <sub>2</sub> =1.51	E1 <b>=2.20</b>	E <sub>2</sub> =1.67
LUMO=-3.683	E=2	2.59	E=	1.72	E=	1.94

	؞ۑۿۑۿۑۿۑ <sup>ڡ</sup> ؞ۿۑۿۑۿۑۿ	းမွန်မွန်မှုန် မွန်မွန်မှုန်	ىيىقىيقى قوي يەرەقچە يەرە	ىقىقىقىقى. بۇيغىقى ق	းမွန်မွန်မှုန် ၂နမ္ခန်မှုန်မှုန်	- 4 4 4 4 <b>4 7</b> - 4 4 4 4 4 5 - 4 4 4 4 4 5
	BE1 <b>=-85.1</b>	BE2=- <b>59.0</b>	BE1 <b>=-62.3</b>	BE2 <b>=-39.0</b>	BE1 <b>=-64.0</b>	BE2 <b>=-42.9</b>
1,2-AQ	E1= <b>3.28</b>	E <sub>2</sub> =2.17	E1=2.33	E <sub>2</sub> =1.30	E1= <b>2.44</b>	E2=1.47
LUMO= <b>-3.298</b>	E=2	2.73	E=	1.82	E=	1.95
	، پۇيۇرۇر. ، ئوغۇم.	، وغريقو م ، موقو موقر ، موقو موقر	မ သွမ်းမွမ်းမွမ ျမ်းမွမ်းမွမ်း	ې پې شي شي کې په يې شي شي کې په يې شي کې	ې د وقوقو قو رقوقو قو	۵ پیڅی څي څي په چې څي څي ه
1,4-AQ	BE1 <b>=-60.2</b>	BE2 <b>=-60.4</b>	BE1 <b>=-41.2</b>	BE2= <b>-33.3</b>	BE1 <b>=-47.0</b>	BE2 <b>=-37.1</b>
LUMO=3.257	E <sub>1</sub> =2.31	E <sub>2</sub> =2.23	E <sub>1</sub> =1.54	E <sub>2</sub> =1.17	E <sub>1</sub> =1.80	E <sub>2</sub> =1.31
	E=2	2.27	E=	1.36	E=	1.56
	မှ မွန်မွန်မှုန်မှုန် မွန်မွန်မှုန်မှုန်	ې پوغونوني پغونونونې پ	မ သွမ်သွမ်သူမီသူ သမ္မာမီသွမ်သွမ်သ	ى ئى ئى يەرىمى مى يەرىمى مى	ې بېغونونو د. مونونو کې	ې پوغوغونې موغوغونې ف
1,5-AQ	BE1 <b>=-77.4</b>	BE2= <b>-71.9</b>	BE1 <b>=-57.8</b>	BE2 <b>=-48.3</b>	BE1 <b>=-63.4</b>	BE2= <b>-53.4</b>
LUMO=-3 990	E1 <b>=3.05</b>	E <sub>2</sub> =2.71	E <sub>1</sub> =2.25	E <sub>2</sub> =1.86	E <sub>1</sub> =2.50	E2=1.98
	E=2		E=2.05		E=:	2.24
l L L L	دوقو وقو قو رقو قو قو قو	ۥ؞ڡؖؖۑ؞ٞۅ؞ڡۛۑ؋ ؞؋ۑؚ؋ۑؚ؋ۑؚ؋ۑ؋	ې دوغوغوغوغو دغوغوغوغر	دوقو وقوقو دقوقو وقوقو دقوقو وقوقو	ە بەرۋەرۋەرۋە بەرۋەرۋەرۋەر	م درفرغرغوم دفوغوغوفر
1,7-AQ	BE1 <b>=-78.4</b>	BE2= <b>-70.4</b>	BE1 <b>=-58.6</b>	BE2= <b>-46.7</b>	BE1 <b>=-64.2</b>	BE2= <b>-50.9</b>
LUMO= <b>-3.964</b>	E <sub>1</sub> =3.07	E <sub>2</sub> =2.65	E <sub>1</sub> =2.27	E <sub>2</sub> =1.63	E <sub>1</sub> =2.52	E2=1.87
	E=2.86		E=1.95		E=2.19	
	ၖမွမ်းမွမ်းမွမ်း ၂မ်င္မမ်င္မမ်င္မမ်င္မ	ႋမွမိမွမိမွမိမွမ် ၂မိမ္မမိမွမ်မွမ် ၂မိမ္မမ်မွမ်မွမ်	؞ۑڠۑڠۑڠۑۿۅ ؞ڠۑۣڠۑۣۼۑۼ	ၖၜၜၴၜၜၜၜၜၜ ၟၜၜၟၜၜၟၜၜၟၜ	ၖမိမမိမမိမ ၂မိမ္မမိမွမ်မှ ၂မိမ္မမိမွမ်မှ	وي قي قي قي د روي قي قي قي روي قي قي ق
2,3-AQ	BE1 <b>=-104.8</b>	BE2= <b>-74.5</b>	BE1=-81.1	BE2= <b>-56.1</b>	BE1= <b>-83.0</b>	BE2 <b>=-60.1</b>
LUMO=-4.274	E <sub>1</sub> =4.17	E <sub>2</sub> =2.77	E1= <b>3.20</b>	E2=1.98	E1= <b>3.32</b>	E <sub>2</sub> =2.16
	E=3	5.47	E=	2.59	E=	2.74

0		းမွှစ်မွှစ်မွှစ်မွှစ် မွှစ်မွှစ်မွှစ်မှုစ်မ	းမှန်မှန်မှန်မှုစ စန်မှုန်မှုန်မှုစ်	، يەرەپەرە، رەپەرەپەرە،	، يۆچۈچۈچە مەيغوغوغ،	ىرى ئەرىقى ئەرە ھەرە ئەرە ئەرە يەرە يەرە يەرە يەرە يەرە ي
	BE1=-75.7	BE2=-71.7	BE1 <b>=-56.2</b>	BE2= <b>-47.4</b>	BE1=-62.0	BE2=-51.4
2,6-AQ	E1 <b>=2.97</b>	E2=2.69	E1 <b>=2.18</b>	E <sub>2</sub> =1.71	E1 <b>=2.44</b>	E2=1.90
LUMO= <b>-3.935</b>	E=2	2.83	E=	1.95	E=:	2.17
	းမွန်မွန်မွန်မွန ကိမ္မခံမွန်မွန်	- يەقرىقى قورىغى - يەۋرىقى قورىغى - يەۋرىقى قورىغى	း လိုလ္ရမ်ိဳ လွမ်ိဳလွမ် ၂မိုလ္မမ်ိဳလွမ်ိဳလွမ်ိဳး ၂မိုလ္မမ်ိဳလွမ်ိဳလွမ်ိဳး	- يەڭرىكى - يەڭرىكى يەڭ - يەڭرىكى يەڭرىكى	، بغرية رومه روموموم،	؞ۑڡٚۑڡؖٚ؈ڡٚؿ ؞ڡٚڕڡ۫ڕڡ۫ڕڡٚ
29-40	BE1=- <b>71.1</b>	BE <sub>2</sub> =-62.4	BE1 <b>=-50.3</b>	BE <sub>2</sub> =-41.8	BE1=- <b>57.2</b>	BE <sub>2</sub> =-44.4
2,7-AQ	E1 <b>=2.76</b>	E <sub>2</sub> =2.32	E1 <b>=1.89</b>	E <sub>2</sub> =1.44	E1=2.21	E <sub>2</sub> =1.53
LUMO= <b>-3.617</b>	E=2	2.54	E=	1.67	E=	1.87
	မ္မာရိန္အရိန္အရန္ ၂ရမ္မာရန္အရန္	ې د څې څې څې د چه چه چه ر ف	မ သွန်သွန်သွန်သ သိမ္မာဆိုရှိသည်	ىرىقى قۇرۇ يەرە يەقى قۇرۇ يەرە يەقى قۇرۇ	ۅ ؠؿڣۑڣۑڣؠ ؠڣۑڣۑڣ	م بقي قي قي ت بقي قي قي قي ف
9,10-AQ	BE1=-55.1	BE2= <b>-56.5</b>	BE1= <b>-36.1</b>	BE2= <b>-29.0</b>	BE1= <b>-41.9</b>	BE2= <b>-34.5</b>
LUMO=-3.083	E1= <b>2.08</b>	E <sub>2</sub> =2.07	E1=1.33	E2 <b>=0.84</b>	E1=1.58	E <sub>2</sub> =1.23
2000 3.000	E=2.08		E=1.08		E=	1.41
	, 8-9, 3 9-9, 9-9, 9-9, 9-9, 9-9, 9-9,	●20 → 20 → 20		900 - 1 900 - 1 900 - 90 900 - 90 900 - 90		90 190 190 190 190 190 190
	BE1 <b>=-84.9</b>	BE2= <b>-59.8</b>	BE1 <b>=-62.2</b>	BE2= <b>-39.7</b>	BE1 <b>=-63.9</b>	BE2= <b>-43.6</b>
9,10-PQ	E1= <b>3.28</b>	E <sub>2</sub> =2.19	E <sub>1</sub> =2.33	E <sub>2</sub> =1.33	E1= <b>2.44</b>	E2=1.50
LUMO=-3.312	E=2.74		E=1.83		E=1.97	
	دور می رفت می می می رفت می می می رفت می می	دوه و رف و ف و ف و د رف و ف و ف و د رف و ف و ف و	رو <b>گره</b> رقبوقوقود رقبوقوقو	دو قام دو قوم دقو قوقود دقو قوقود	دوقوم دوقوم دقوقوقود دقوقوقود	
3.4-PO	BE1= <b>-89.6</b>	BE2 <b>=-63.8</b>	BE1 <b>=-66.6</b>	BE2 <b>=-43.8</b>	BE1 <b>=-68.5</b>	BE2 <b>=-47.3</b>
5,4-rQ	E1= <b>3.45</b>	E <sub>2</sub> =2.36	E1 <b>=2.49</b>	E <sub>2</sub> =1.50	E1 <b>=2.60</b>	E2 <b>=1.66</b>
LUMO=-3.543	E=2	2.91	E=	2.00	E=	2.13

	င္ၿမိဳင္ၿ <sup>6</sup> ိ စမိဳင္ၿမိဳင္ၿမိဳင္ ငမိစ္ၿမိဳင္ၿမိဳင္	دوقو <sup>ق</sup> دوقوقو دقوقوقو دقوقوقو	دوقوم • فوقوقود دقوقوقور	دوقوق موتوتوفود وقوتوفوذ	င္ၿမိဳ႕ စမိဳ႕မိဳ႕မိဳ႕ ငမိဳ႕မိဳ႕မိဳ႕	ေနိုင်ငံ ရောင်နေရင် ကိုန်ရောင်
1,4-PQ	BE1 <b>= -63.8</b>	BE2 <b>=-62.6</b>	BE1 <b>=-45.0</b>	BE2 <b>=-36.4</b>	BE1 <b>=-50.9</b>	BE2 <b>=-41.1</b>
LUMO= <b>-3.485</b>	E <sub>1</sub> =2.43	E <sub>2</sub> =2.34	E <sub>1</sub> =1.67	E <sub>2</sub> =1.17	E1 <b>=1.95</b>	E <sub>2</sub> =1.40
	E=2	2.39	E=	1.42	E=	1.67



Fig. S1 CV curves of first cycle at 0.1 mV s<sup>-1</sup> of 1,4-BQ, 1,4-NQ and 9,10-AQ.

		Voltage (V vs Li	-+/Li)	
System		Theo.		Expt.
	lc-wpbe/6-311+g(d,p)	wb97x/6-311+g(d,p)	b3lyp/6-311+g(d,p)	
1,4 <b>-</b> BQ	2.59	2.67	2.55	2.41
1,4 <b>-</b> NQ	2.35	2.43	2.33	2.40
9,10-AQ	2.05	2.12	2.08	2.21

**Table S2**. Comparison between experimental voltages and the theoretical voltages of 1,4-BQ, 1,4-NQ and 9,10-AQ calculated by different levels of theory.

	Volta	ge (V vs Li <sup>+</sup> /Li)
System	Theo.	Expt.
1,4-benzoquinone (1,4-BQ)	2.55	2.41
1,4-naphthoquinone (1,4-NQ)	2.33	2.40
9,10-anthraquinone (9,10-AQ)	2.08	2.21
9,10-phenanthraquinone (9,10-PQ)	2.74	$2.72^{a}$
5,7,12,14-pentacenetetrone (PT)	2.00	$2.22^{b}$
2,2'-bi(1,4-naphthoquinone) (BNQ)	2.56	2.45 <sup>c</sup>
1,4,5,8-phenanthrenediquinone (PADQ)	2.68	$2.63^{d}$
pyrene-4,5,9,10-tetraone (PTQ)	2.75	2.59 <sup>e</sup>
5,12-naph-thacenequinone (NAQ)	1.99	2.20 <sup>f</sup>
1,2-benzanthraquinone (BAQ)	2.08	~2.3 <sup>g</sup>

 Table S3. Comparison between the theoretical and experimental voltages.

*a-j*Experimental data from <sup>[1]</sup> Yao et al.,<sup>[2]</sup> Chen et al.,<sup>[3]</sup> Chen et al.,<sup>[4]</sup> and Chen et al.,<sup>[5]</sup> respectively. *<sup>i</sup>j*Experimental data from Cho et al.<sup>[6]</sup>

To examine the reliability of the results, we calculated the energies of the lowest unoccupied molecular orbitals (LUMO) for each neutral molecule and radical anion, which is directly related to the acceptance of electrons.<sup>7</sup> As shown in Figure S1 of Supporting Information, all neutral molecules can obtain electrons from Li<sup>+</sup>/Li redox couple (-1.36 eV) because all of LUMO levels are located from -4.27 to -3.08 eV, while radical anions cannot get more electrons because of higher LUMO levels, which are located from 1.10 to 2.90 eV. Therefore, all the parent quinone molecules can only bear two electrons in their structure.



Fig. S2 Calculated HOMO/LUMO level of neutral molecules and dianions (in eV).



**Fig. S3** Calculated VEA under vacuum condition of neutral molecules, radical anions, dianions, and radical trianions of different isomers.



**Fig. S4** Calculated the first and second voltage plateau for all the isomers of BQs (red), NQs (green), AQs (blue), and PQs (purple) in sodium-ion batteries. O, P, and D represents the *ortho*-quinones, *para*-quinones, and *discrete*-quinones, respectively.



**Fig. S5** Calculated the first and second voltage plateau for all the isomers of BQs (red), NQs (green), AQs (blue), and PQs (purple) in potassium-ion batteries. O, P, and D represents the *ortho*-quinones, *para*-quinones, and *discrete*-quinones, respectively.



Fig. S6 Calculated redox potentials and LUMO energies of 20 parent quinones.



Fig. S7 Calculated average voltages vs Na<sup>+</sup>/Na (red), and K<sup>+</sup>/K (blue) for all the isomers.

System	Theo. (eV)	Expt. (eV)
1,4-benzoquinone (1,4-BQ)	2.17	~2.18
1,4-naphthoquinone (1,4-NQ)	2.00	1.819
9,10-anthraquinone (9,10-AQ)	1.77	1.599

**Table S4.** Comparison of the calculated electron affinities of 1,4-BQ, 1,4-NQ and 9,10-AQ with those of experimental values.

System	E <sub>LUMO</sub> (eV)	VEA (eV)
1,2-NQ	-3.41	-3.19
2,3-NQ	-4.12	-3.74
1,2-AQ	-3.30	-2.99
2,3-AQ	-4.27	-3.95

**Table S5.** The LUMO energy and VEAs of 1,2-NQ, 1,2-AQ, 2,3-NQ and 2,3-AQ.



Fig. S8 Plots of calculated voltages against  $\Delta A_{2Li}$  for a) *para*- and b) *ortho*-quinones.

 $\Delta A_{4Li}$  values for quinones with four carbonyls were also calculated that can go through fourelectron reduction reactions, including 5,7,12,14-pentacenetetrone (PT), 2,2'-bi(1,4naphthoquinone) (BNQ), 1,4,5,8-phenanthrenediquinone (PADQ), and pyrene-4,5,9,10-tetraone (PTQ). Though four data points are not sufficient for a linear fitting, it is clearly seen in Figure S9 that the voltages of these quinones are in positive correlation with their corresponding  $\Delta A_{4Li}$ .



Fig. S9 Calculated voltages variation with  $\Delta A_{4Li}$ .

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