

بِسْمِ اللّٰهِ الرَّحْمٰنِ الرَّحِيمِ



سازمان توسعه منابع ازrثی

اولین همایش ملی باتری لیتیومی

1st National Lithium Battery Conference
(LBC 2021)



بهبود عملکرد باتری های لیتیوم-یون با اصلاح الکترولیت

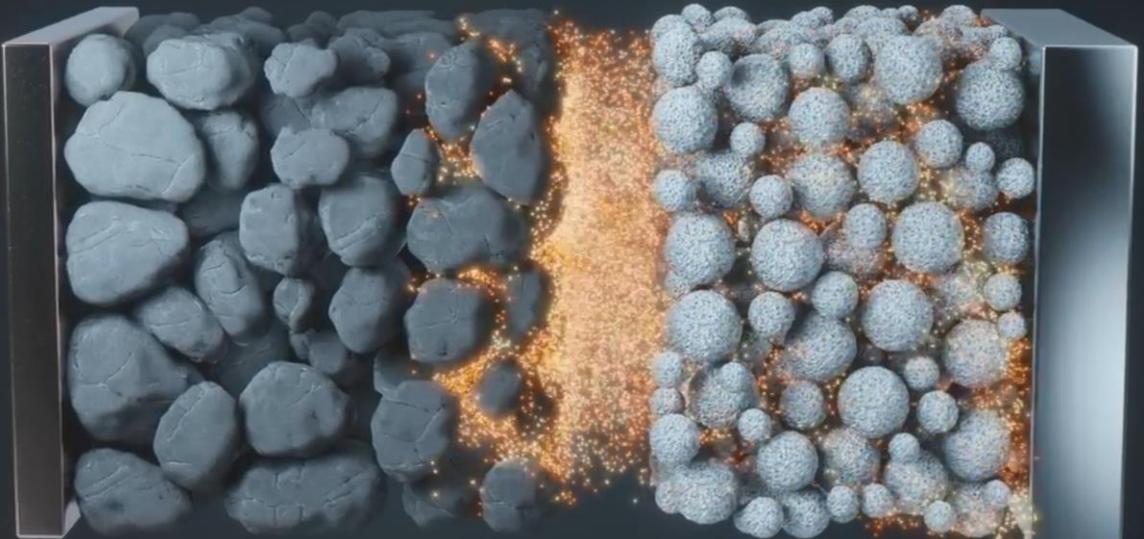
فرشاد بوربور اژدری^{۱*}، ابوالفضل فتح الهی زنوز^{۲*}، حسن شکوهی مهربانی^۲، علی حیدری^۳

^۱ کاشان، دانشگاه کاشان، دانشکده شیمی، گروه شیمی کاربردی

^۲ تهران، قطب باتری لیتیومی کشور

^۳ دانشگاه سیستان و بلوچستان، دانشکده شیمی

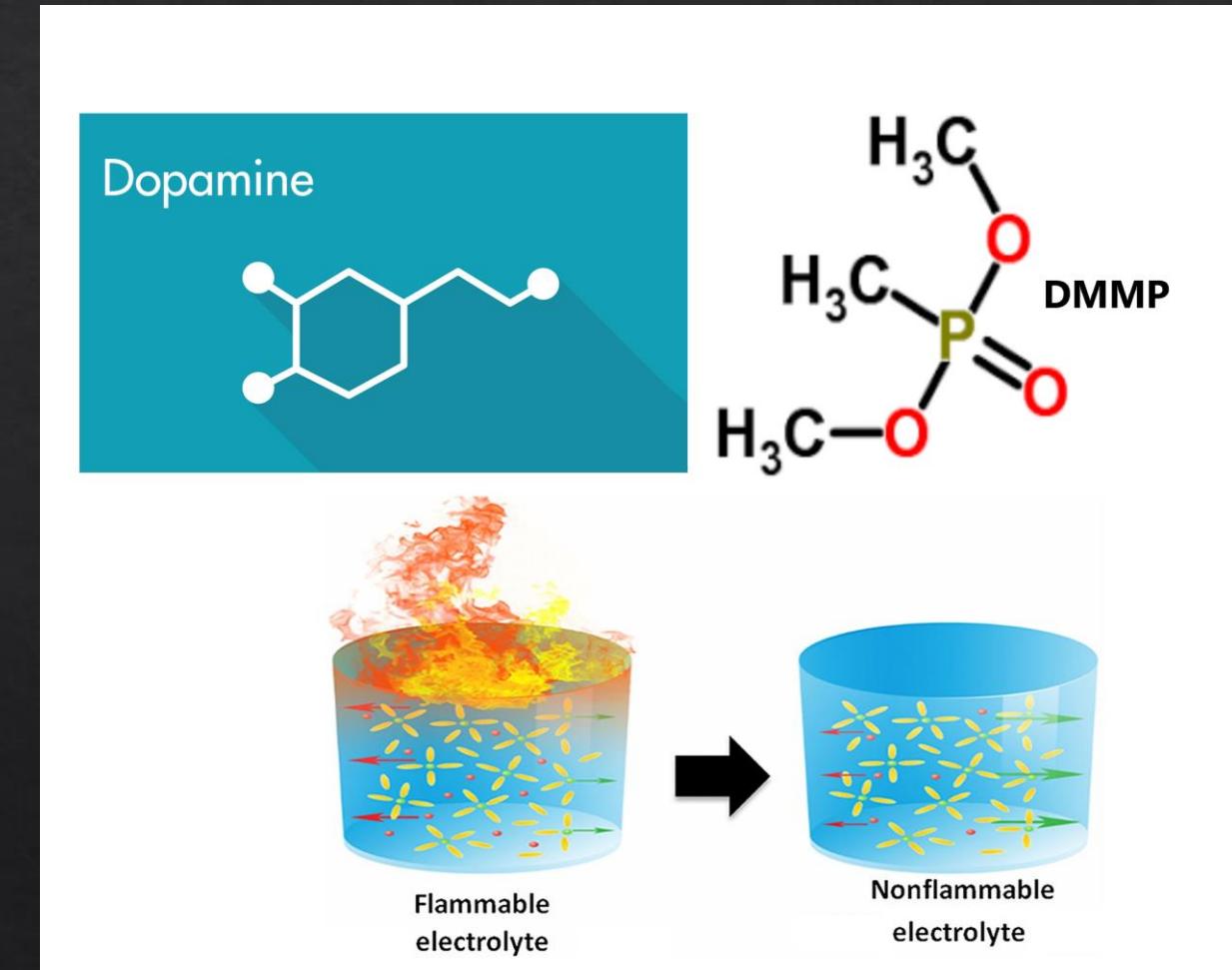
* آدرس ایمیل: farshadborbor.2009@gmail.com



Commercial Electrolyte

+ 5%wt DMMP

+ 0.1%wt Dopamine



The best performance content: Optimized system

Electrolyte *	Cathode	Anode	DMMP	DOP
LiPF6 [1M] (EC:EMC:DMC) (1:1:1)	NMC-532	Graphite	5%wt of *	0.1%wt of *

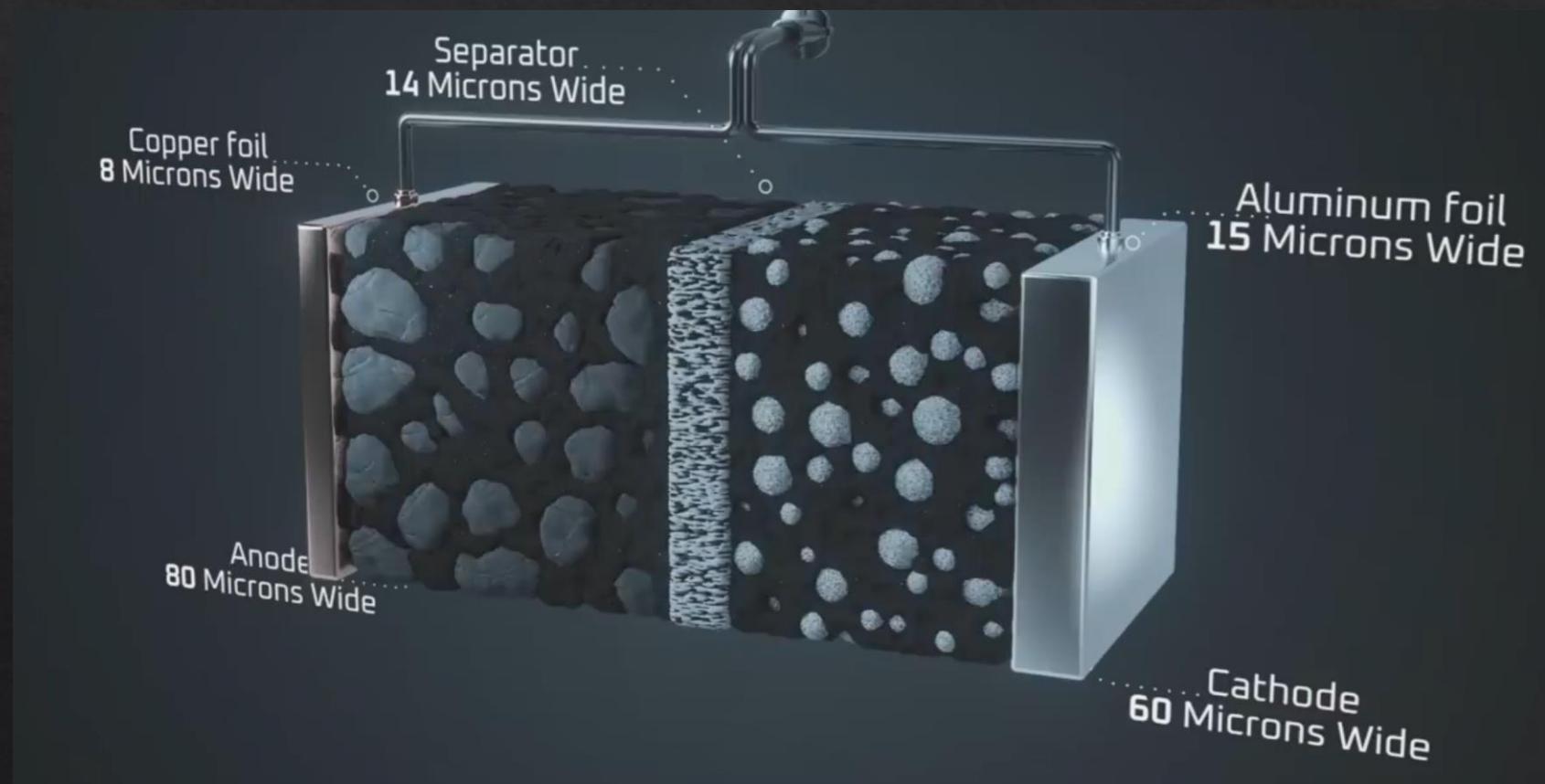


Table 1. Energy levels of DOP compared to DMC, EMC, and EC

	DOP	DMC	EMC	EC
LUMO (eV)	-0.96	1.88	1.40	1.74
HOMO (eV)	-11.60	-12.85	-13.33	-12.90

Table 2. The values of the examined formulations

Sample	formulation	Additive
B	Commercial electrolyte	-
D	Electrolyte + 5%v DMMP	DMMP
0.01DP	Electrolyte + 5% <u>wt</u> DMMP + 0.01% <u>wt</u> DOP	DMMP + DOP
0.05DP	Electrolyte + 5% <u>wt</u> DMMP + 0.05% <u>wt</u> DOP	DMMP + DOP
0.1DP	Electrolyte + 5% <u>wt</u> DMMP + 0.1% <u>wt</u> DOP	DMMP + DOP

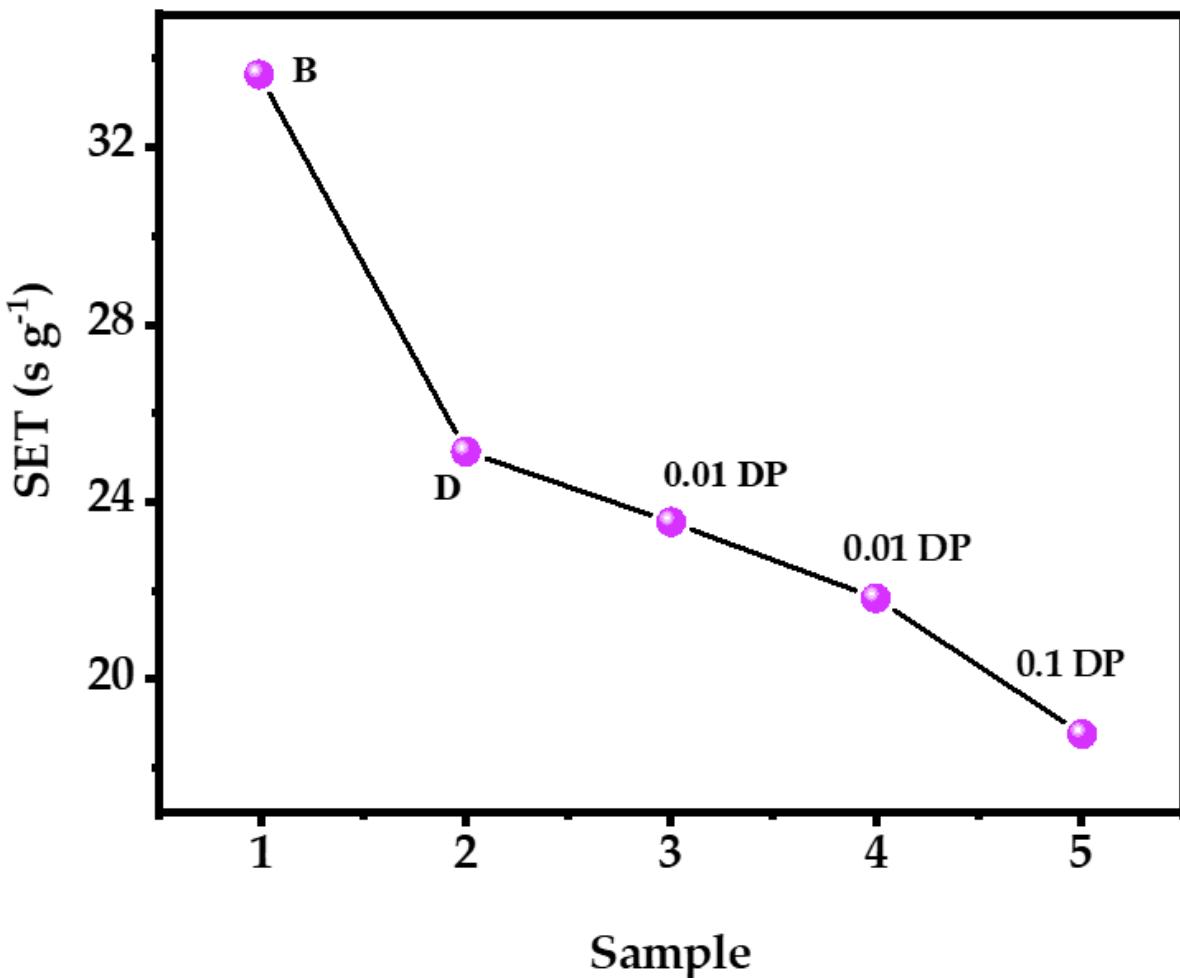
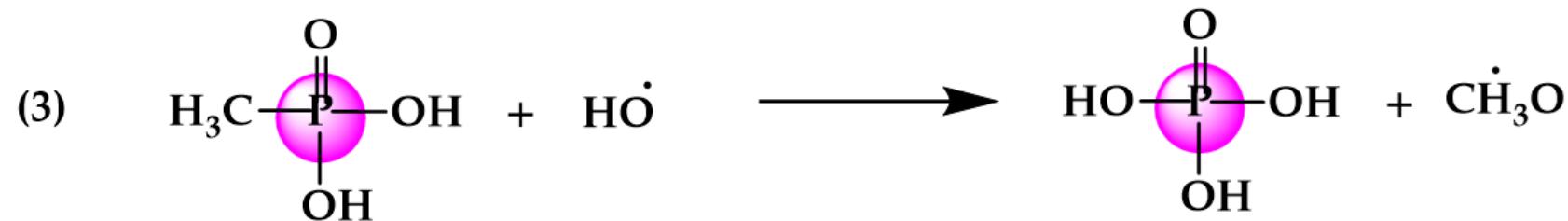
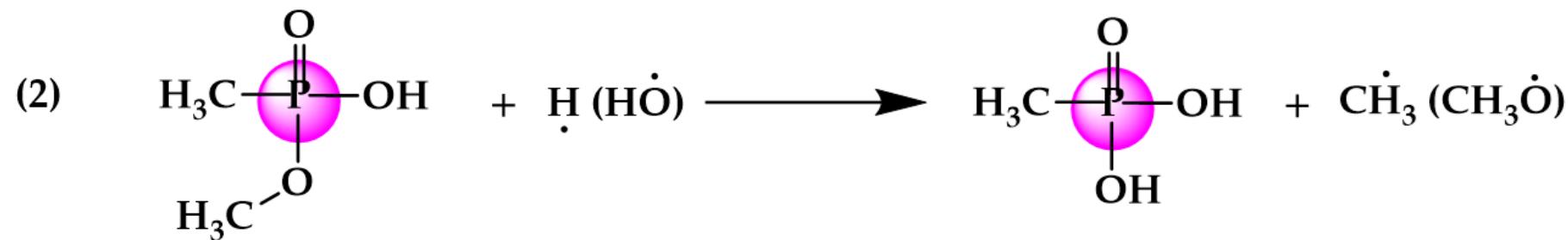
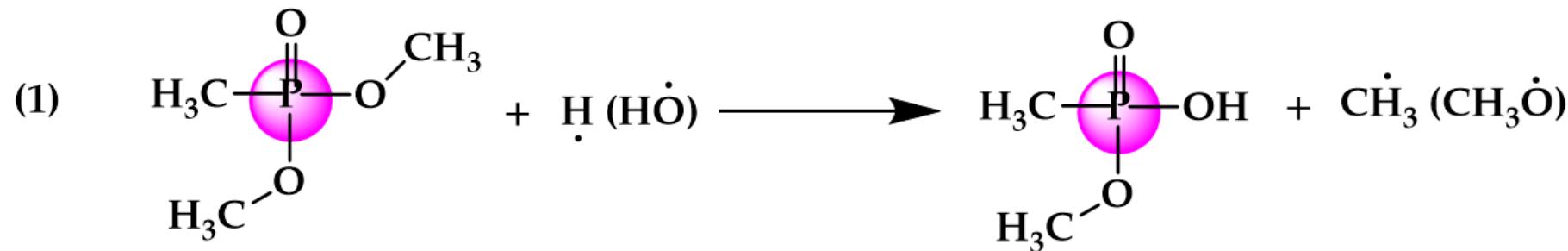


Figure 1. The relationship between the effect of the additive on the flammability of the lithium battery electrolyte



Scheme 1. The possible mechanism for Dimethylmethylphosphonate flame retardant additive.

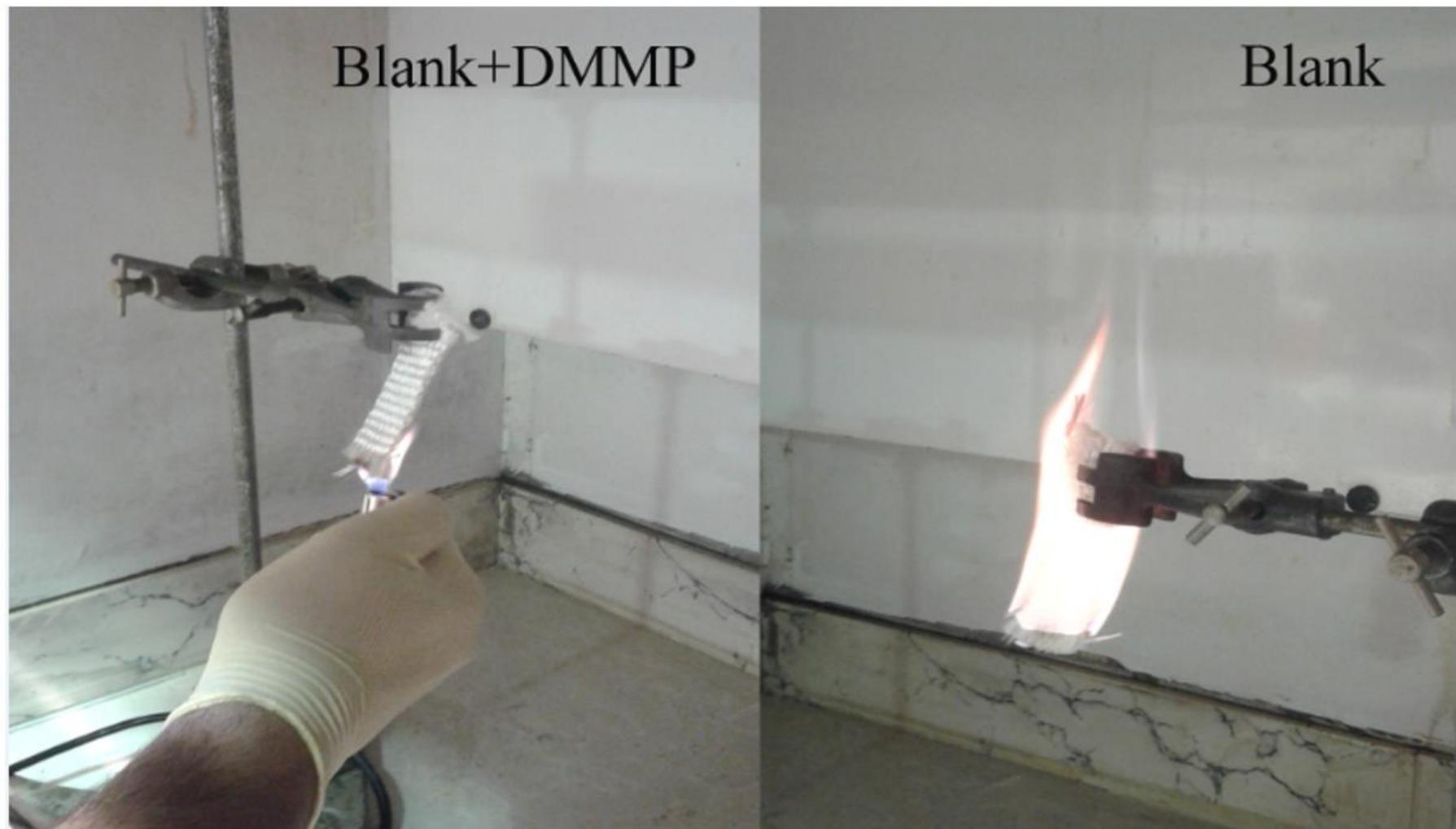


Figure 2. Self-Extinguishing Time (SET) and ignition test of Bare electrolyte (Blank) and resistance of electrolyte with additive of dimethyl methyl phosphonate and dopamine against ignition (0.1DP).

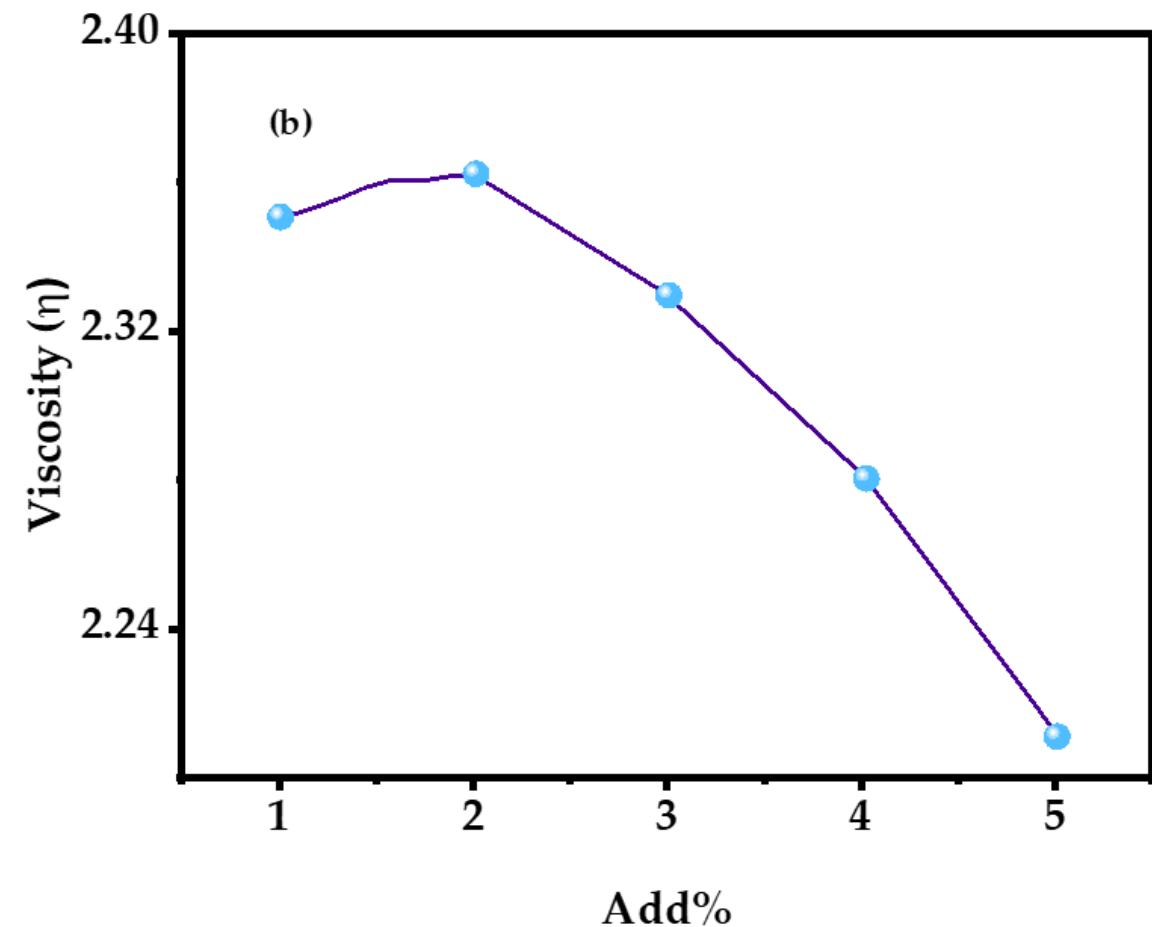
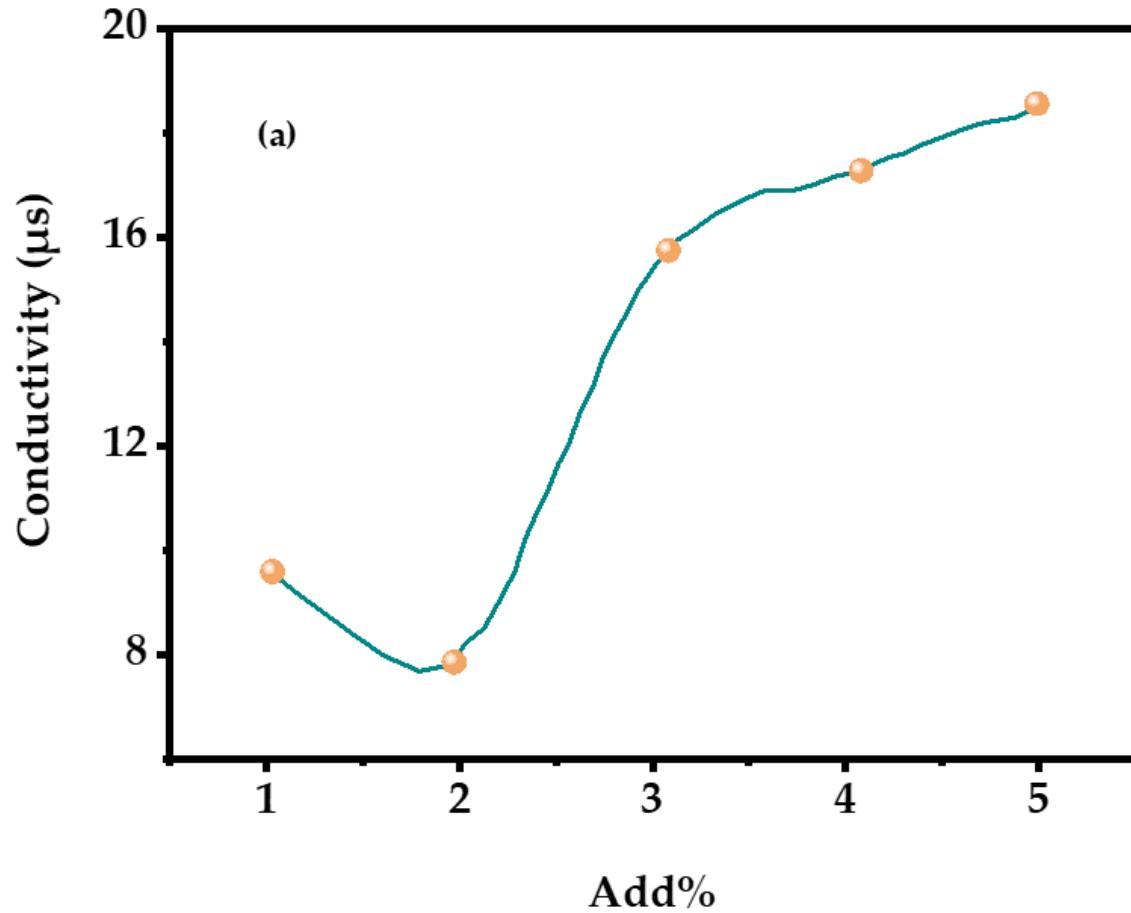


Figure 3. Relationship between variations of conducting (a) and viscosity (b) versus different contents of electrolyte additives.

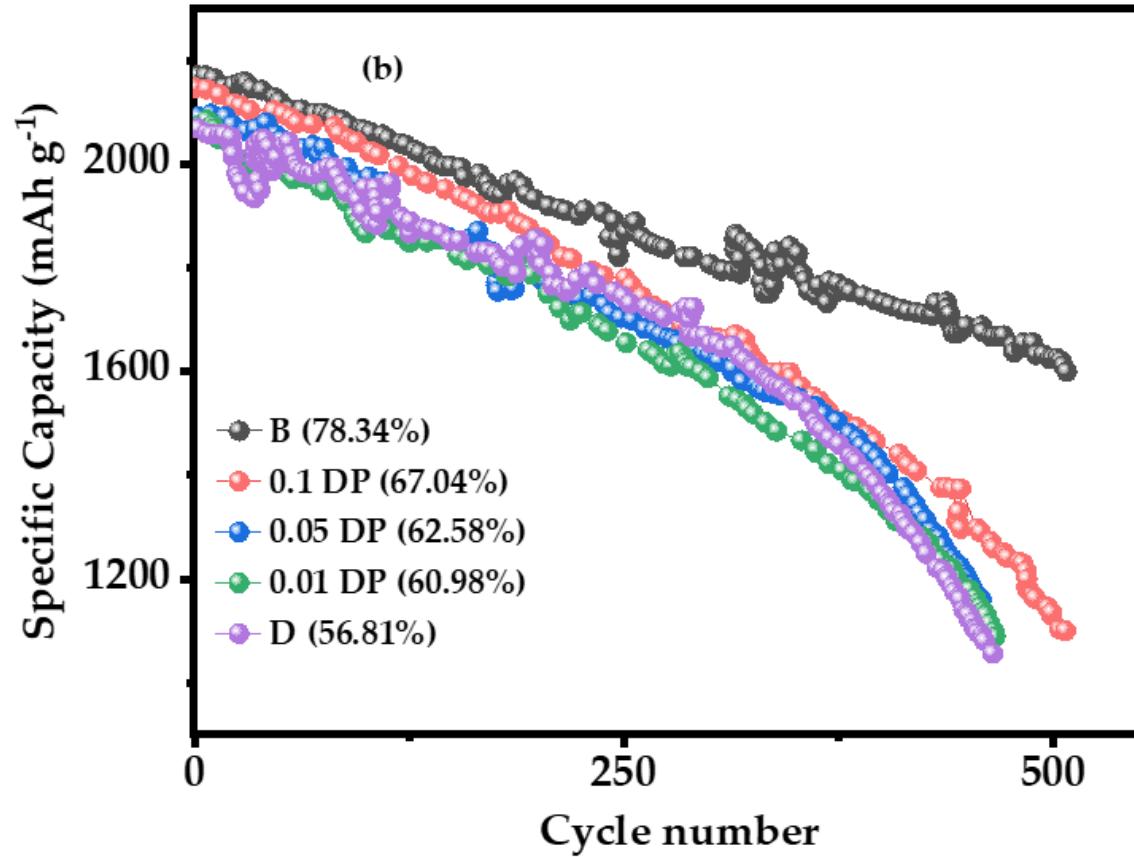
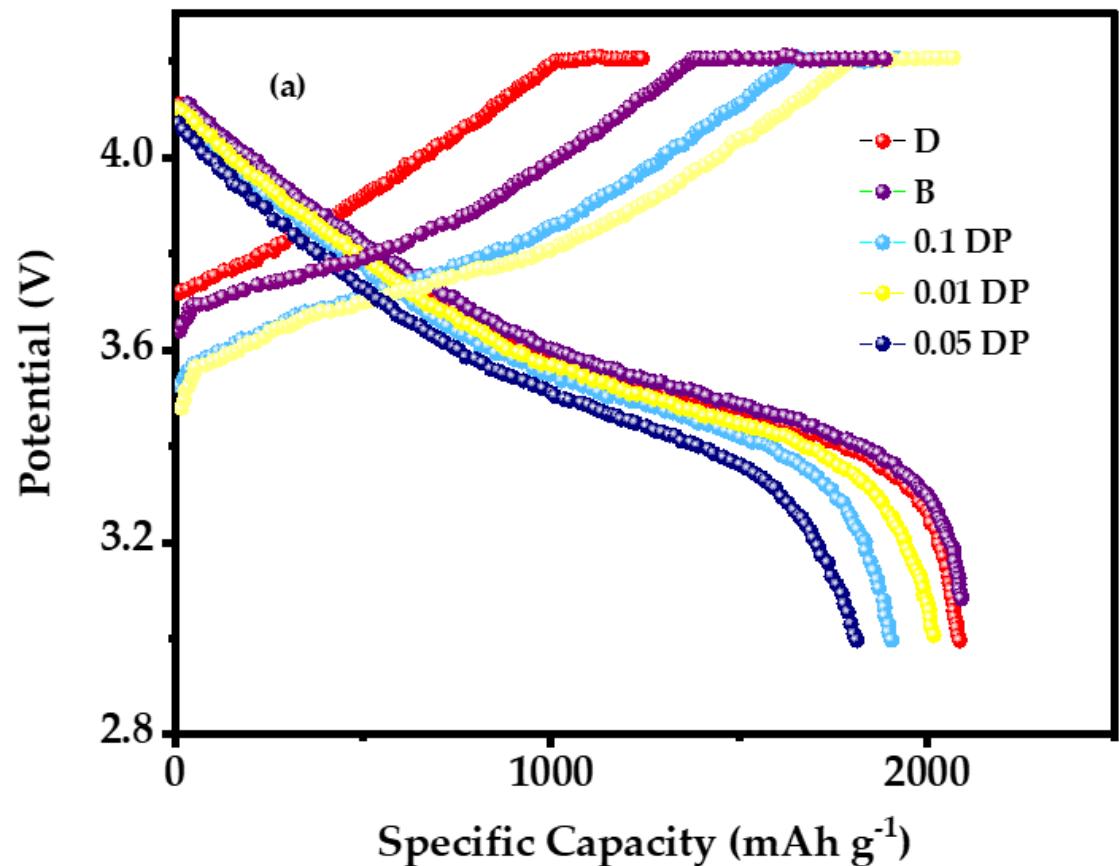


Figure 4. (a) Charging-discharge and (b) Cyclability diagrams for Bare sample and batteries with formulated electrolytes with 5% DMMP and different ratios of dopamine (0.01%wt, 0.05%wt, and 0.1%wt).

Table S4. Charging and discharging capacities of Bare sample compared to the formulated samples.

Sample	Initial charging capacity	Initial discharge capacity	Percentage of reversible capacity
B	2150	2133	99.21
D	2136	2070	96.91
0.01DP	2077	2045	98.21
0.05DP	2096	2068	98.66
0. 1DP	2081	2063	99.14

Table S5. Cyclability data of Bare sample compared to the formulated samples.

Sample	1 st discharge capacity	300 th discharge capacity	capacity loss% after 300 cycles	500 th discharge capacity	capacity loss% after 500 cycles
B	2133	1826	14.39	1671	21.66
D	2070	1589	23.24	1176	43.19
0.01DP	2045	1621	20.73	1247	39.02
0.05DP	2068	1674	19.05	1294	37.42
0. 1DP	2063	1708	17.20	1383	32.96

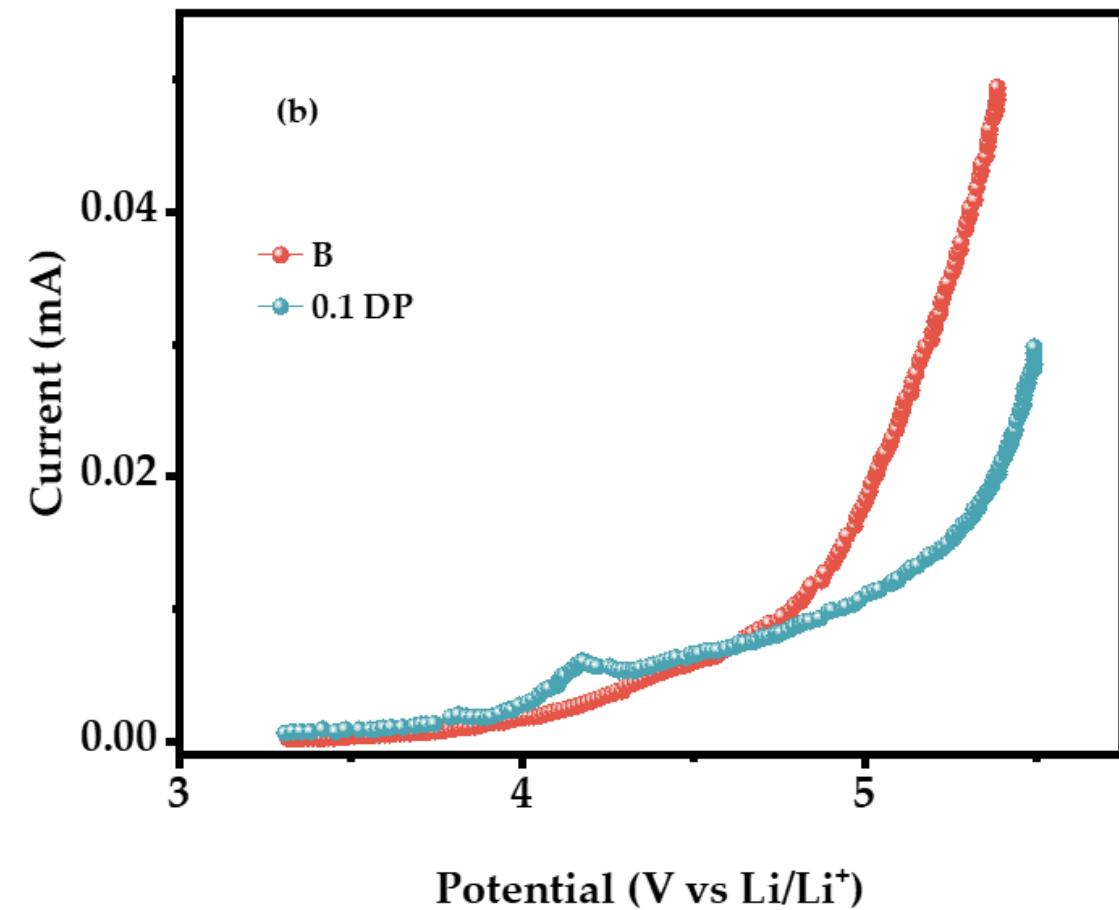
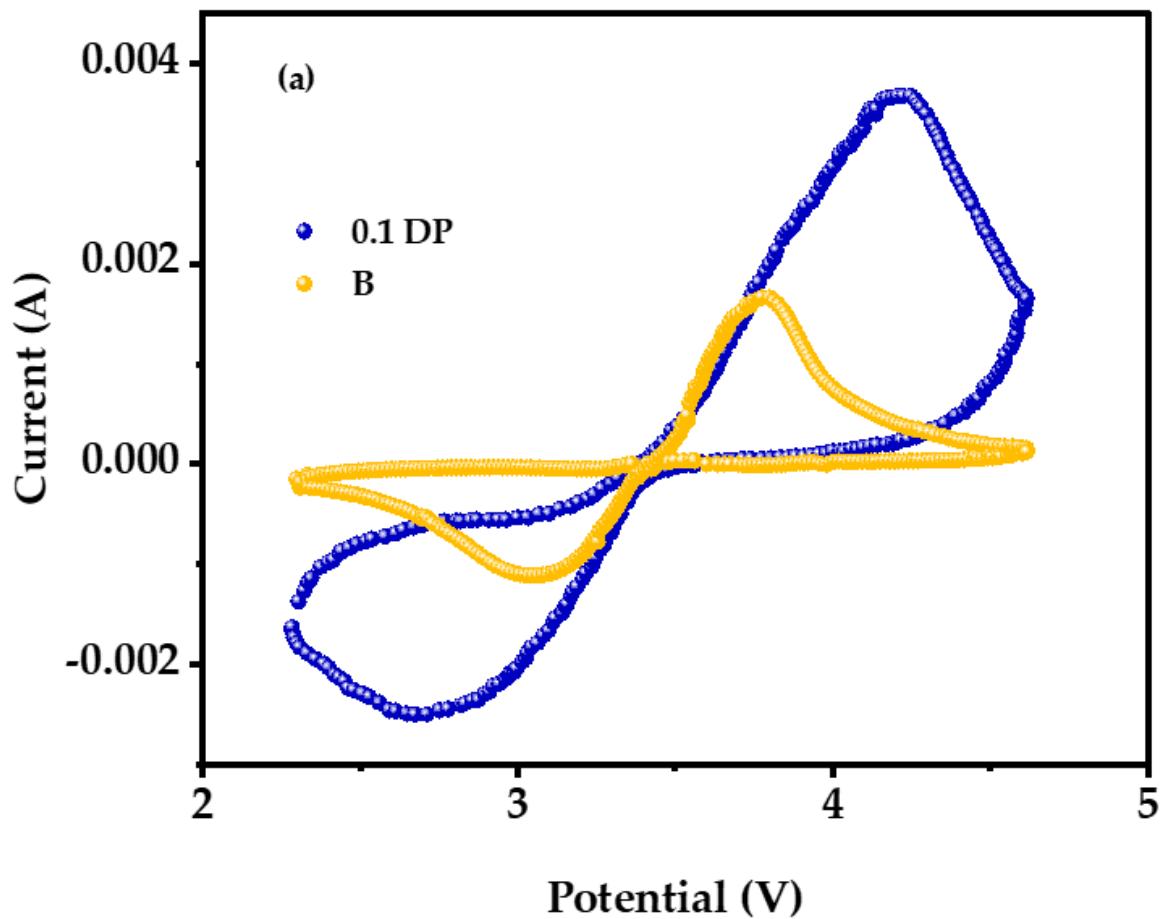


Figure 5. The cyclic voltammetry (a) and LSV (b) plots for Bare sample and DMMP+0.1DOP-containing sample.

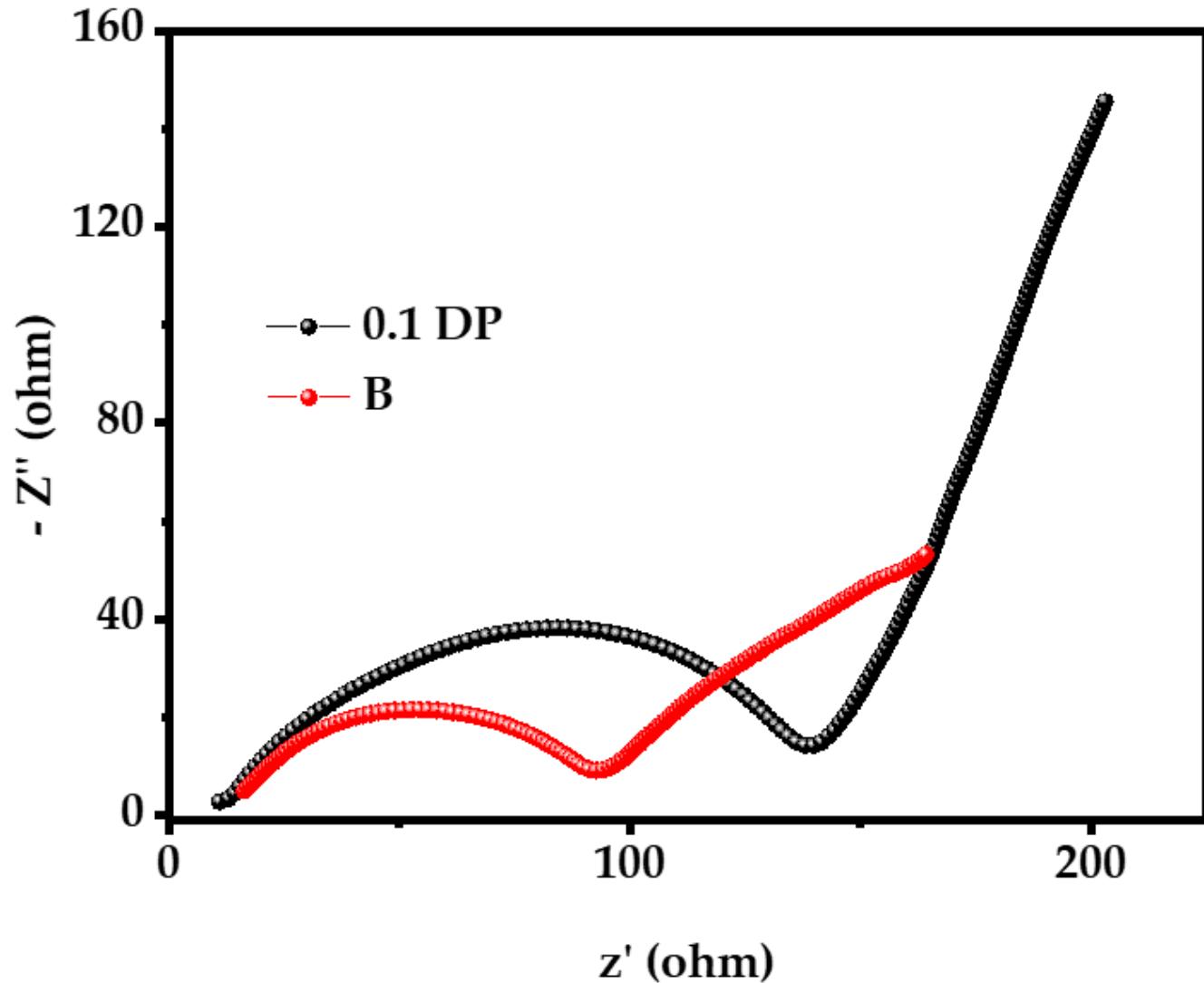


Figure 6. The Nyquist plot for Bare sample and DMMP+0.1DOP-containing sample

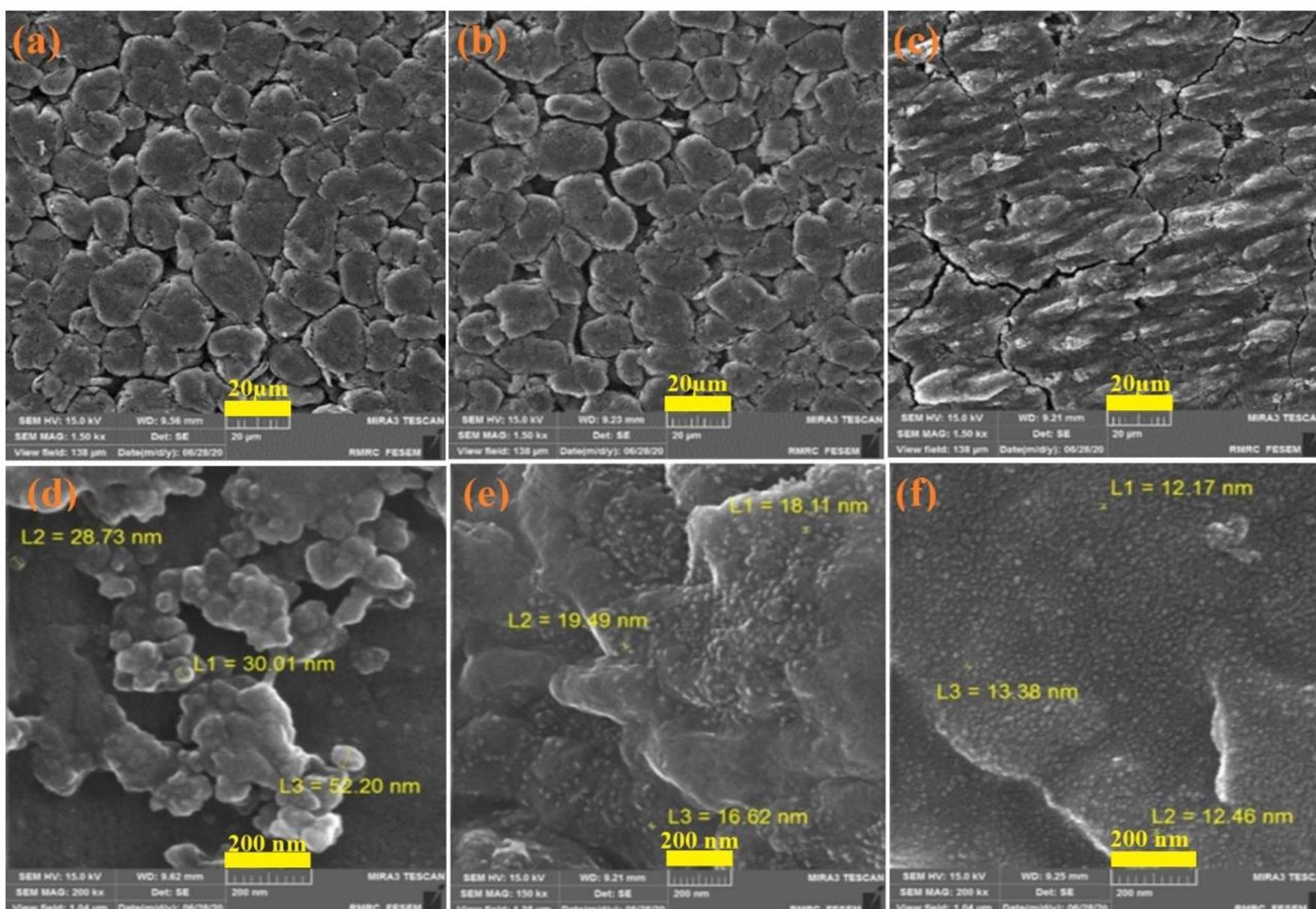
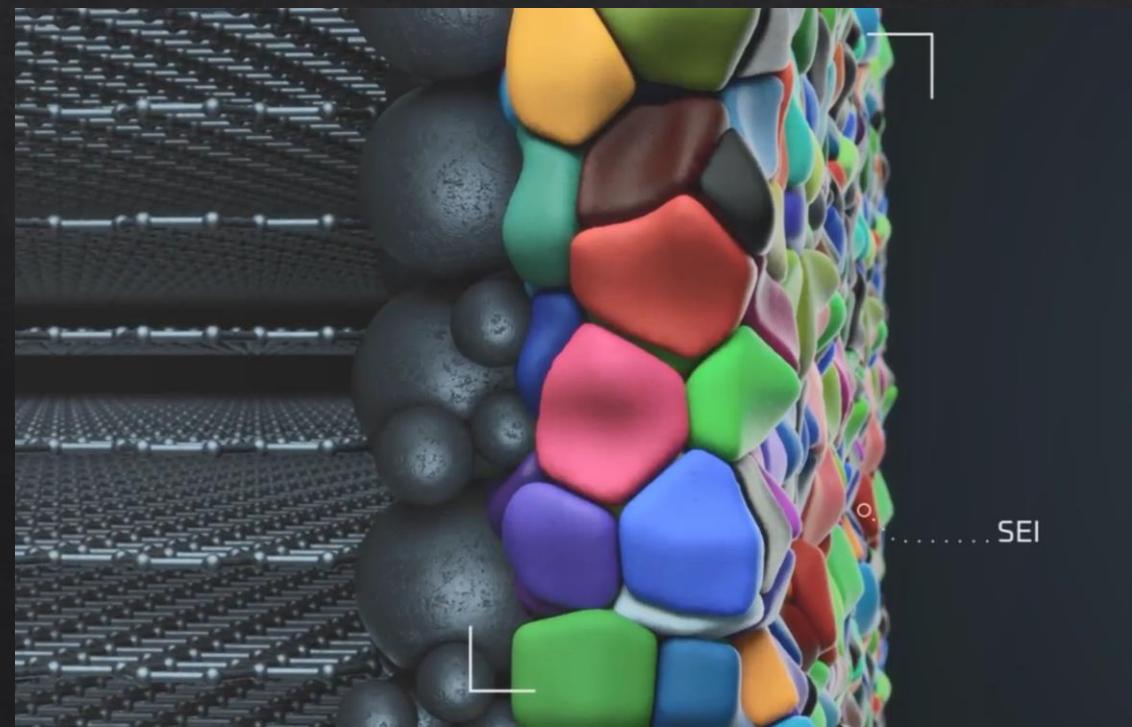
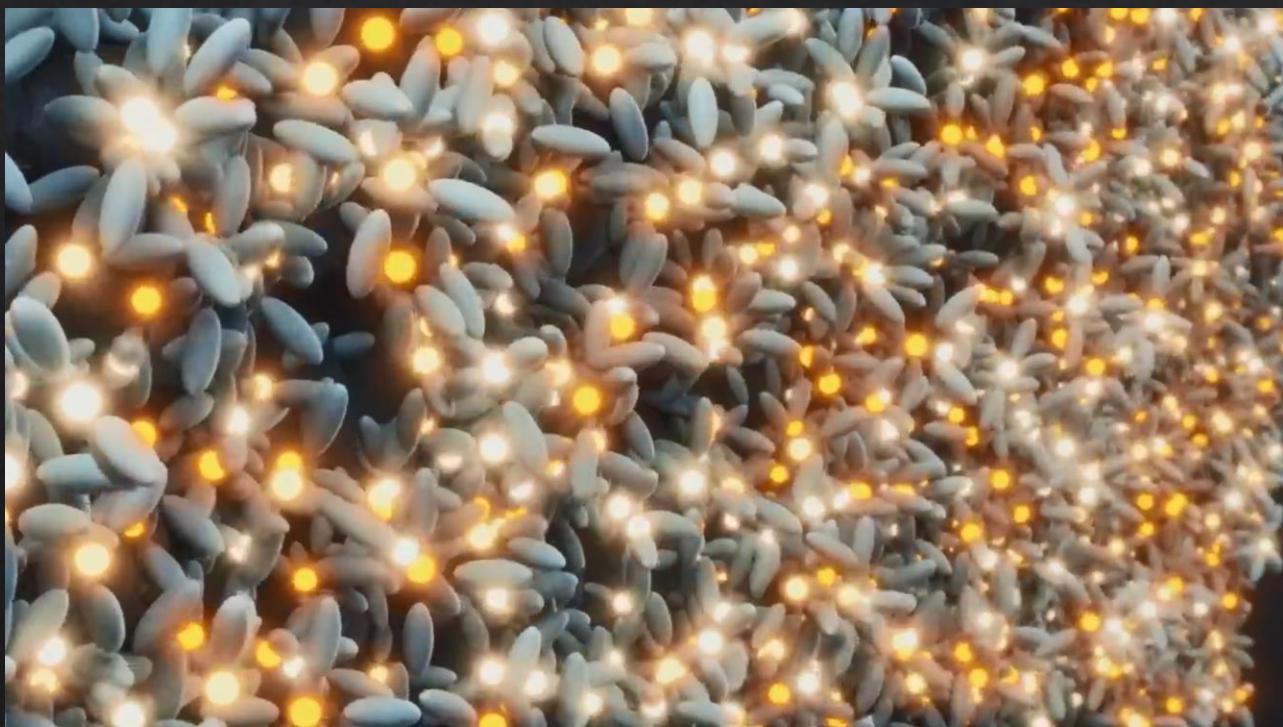
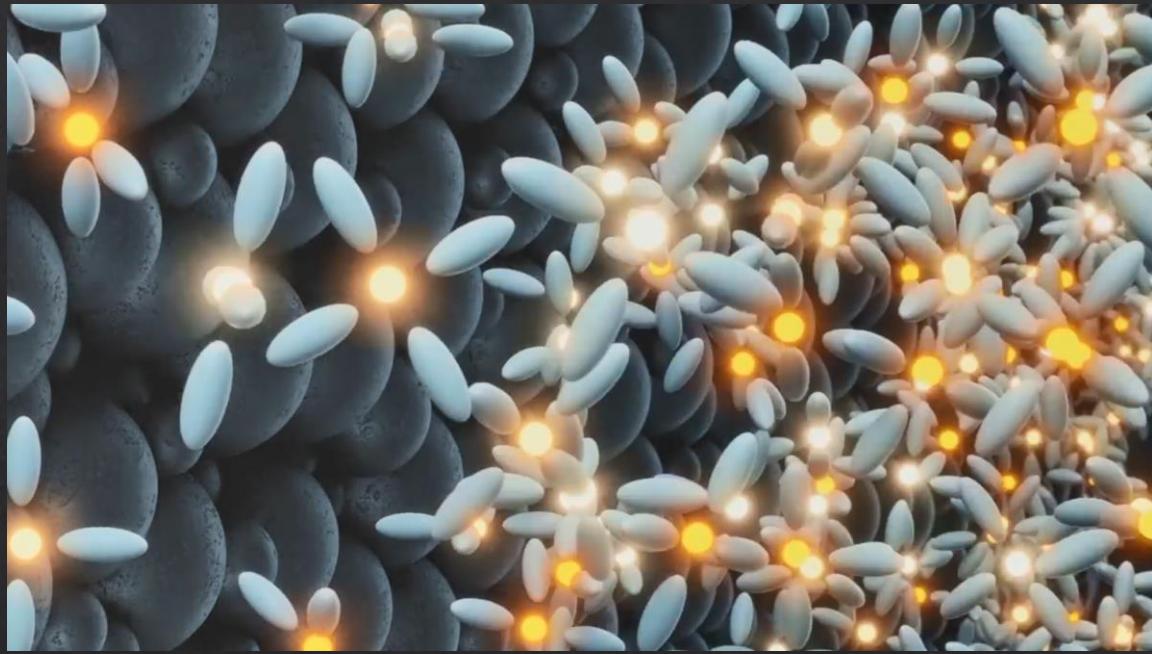
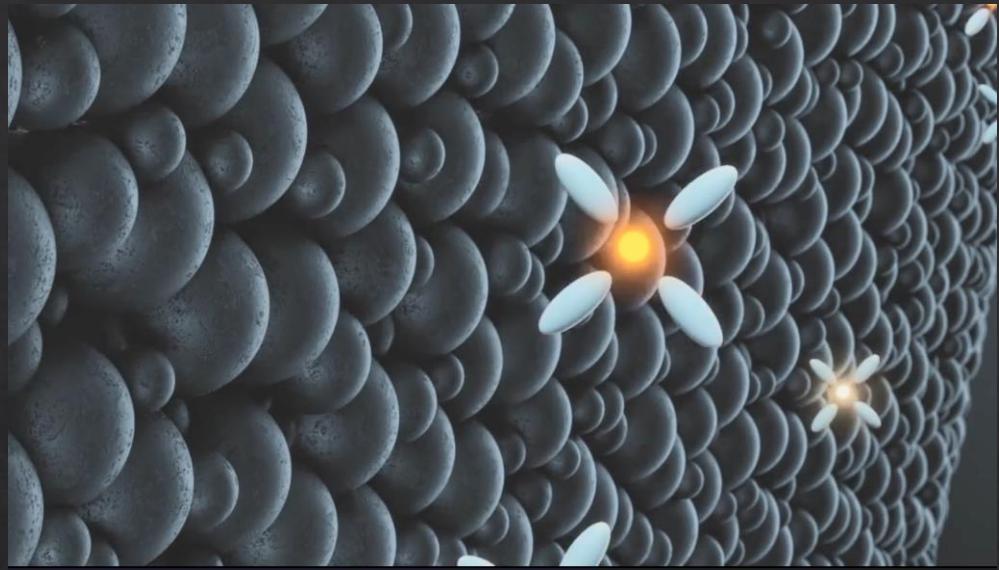


Figure 7. The SEM images of graphite surface for Bare (a), 5%wtDMMP (b), and 5%wtDMMP+0.1DOP (c). And SEM imaged for cathode surface for Bare (d), 5%wtDMMP (e), and 5%wtDMMP+0.1DOP (f).



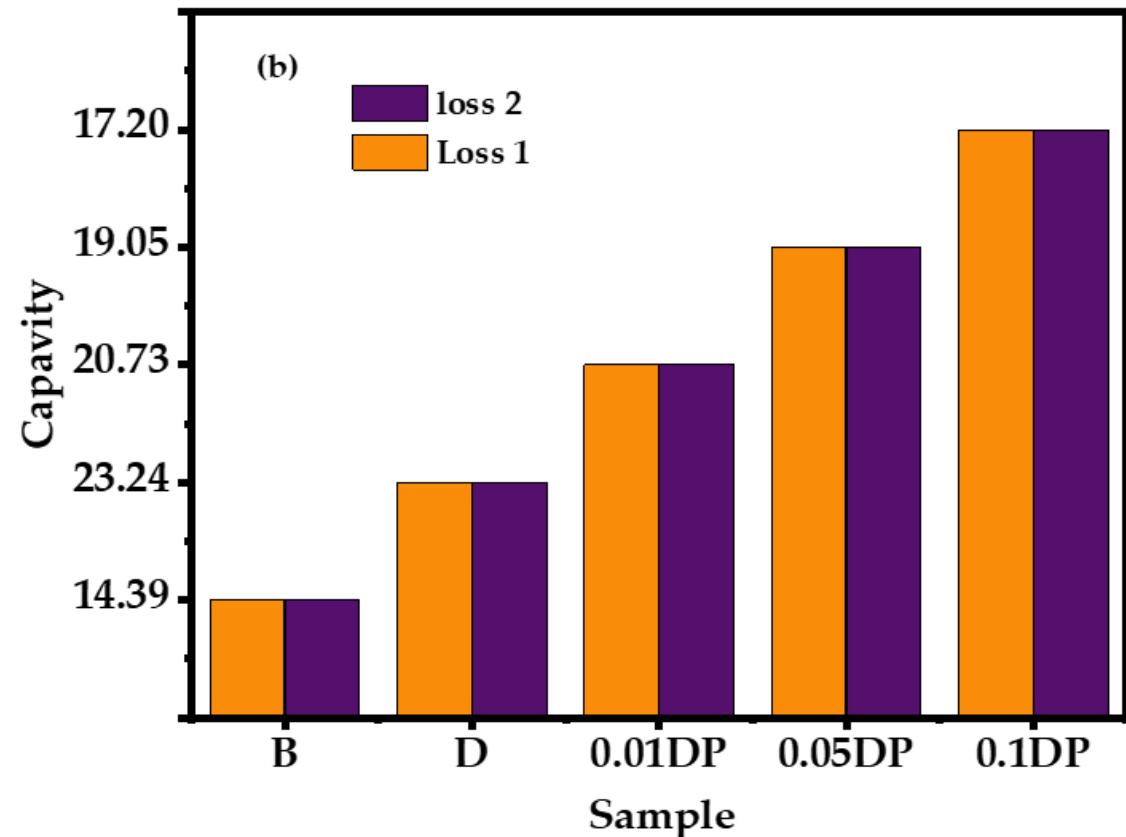
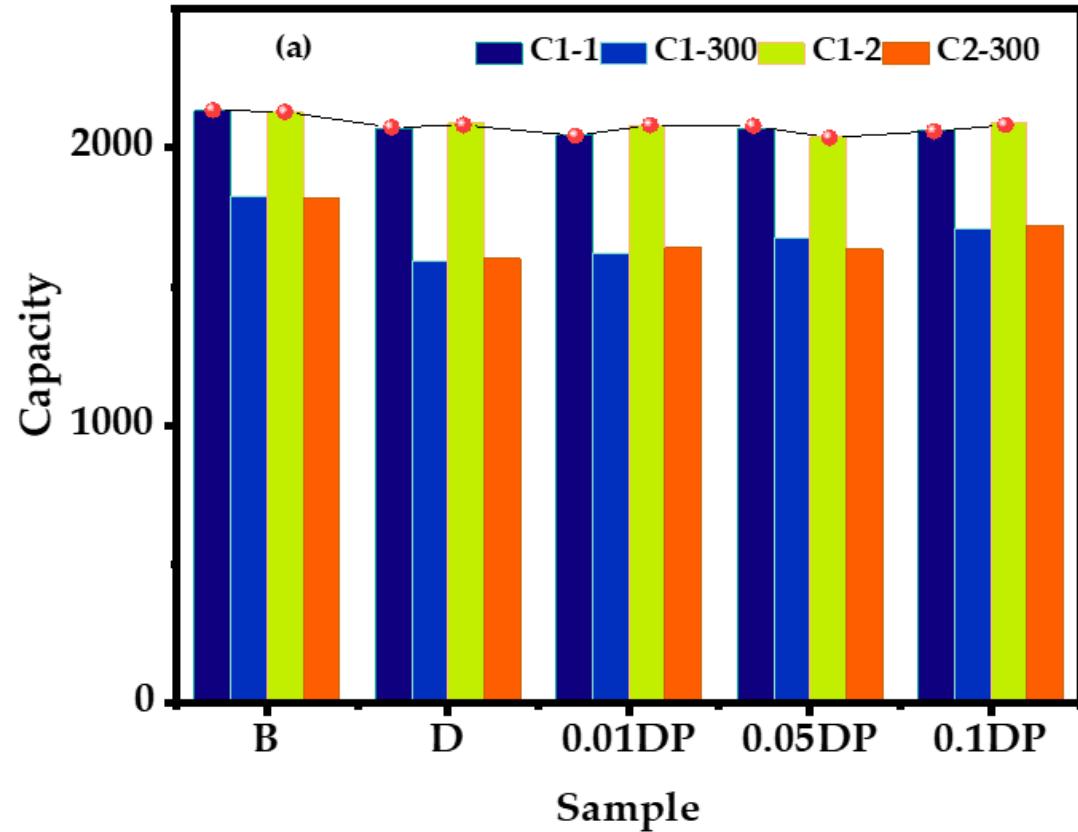


Figure 10. Repeatability of Bare electrolyte cyclicity values and samples with 5% DMMP and dopamine values of 0.01, 0.05 and 0.1% after 300 and 500 cycles.

*C1-1: 1st Discharge capacity of Type 1, C1-2: 1st Discharge capacity of Type 2

*C1-300: 300th Discharge capacity of Type 1, C2-300: 300th Discharge capacity of Type 2

*Loss 1: Capacity loss after 300th cycle for Type 1

*Loss 2: Capacity loss after 300th cycle for Type 2

❖ مراجع:

- ❖ [1] P.V. Chombo, Y. Laoonual, A review of safety strategies of a Li-ion battery, *J. Power Sources*. Vol.**478**, pp. 228649, **2020**.
- ❖ [2] H.-J. Kim, T.N. V Krishna, K. Zeb, V. Rajangam, C.V. V Gopi, S. Sambasivam, K.V.G. Raghavendra, I.M. Obaidat, A comprehensive review of Li-ion battery materials and their recycling techniques, *Electronics*. Vol. **9**, pp. 1161, **2020**.
- ❖ [3] S.S. Zhang, Design aspects of electrolytes for fast charge of Li-ion batteries, *InfoMat.* Vol. **3**, pp. 125–130, **2021**.
- ❖ [4] Y. Qian, S. Hu, X. Zou, Z. Deng, Y. Xu, Z. Cao, Y. Kang, Y. Deng, Q. Shi, K. Xu, How electrolyte additives work in Li-ion batteries, *Energy Storage Mater.* Vol. **20**, pp. 208–215, **2019**.

با تشکر از شما