

Supporting Information

Search map for organic additives and solvents applicable in high-voltage
rechargeable batteries

Min Sik Park,^{*a} Insun Park,^b Yoon-Sok Kang,^b Dongmin Im^b and Seok-Gwang Doo^b

^aComputer-Aided Engineering Group, Samsung Advanced Institute of Technology, Samsung
Electronics, 130 Samsung-ro, Suwon, Gyeonggi-do 443-803, Republic of Korea

^bEnergy Laboratory, Samsung Advanced Institute of Technology, Samsung Electronics, 130
Samsung-ro, Suwon, Gyeonggi-do 443-803, Republic of Korea

* E-mail addresses: ms91.park@samsung.com (M. S. Park)

Table S1 Functional groups included in the molecular descriptor of organic compounds

Category	Functional groups
Oxygen group (11)	alcohol, carbonyl, aldehyde, haloformyl, carbonate ester, carboxyl, ester, methoxy, hydroperoxy, peroxy, ether
Nitrogen group (20)	amide, secondary amine, tertiary amine, primary ketamine, secondary ketamine, primary aldimine, secondary aldimine, imide, azide, azo, cyanate, isocyanate, nitrate, nitrile, isonitrile, nitrosooxy, nitro, nitroso, pyridyl, primary amine
Sulfur group (11)	sulphydryl, sulfide, disulfide, sulfinyl, sulfonyl, sulfino, sulfo, thiocyanate, isothiocyanate, thione, thial
Phosphorus group (4)	phosphine, phosphono, phosphate, phosphodiester
Boron group (4)	borono, boronate, borino, borinate

Table S2 Classification of organic compounds (with $E_{\text{ox}} > 6 V_{\text{Li}}$ and $E_{\text{rd}} < 0 V_{\text{Li}}$) based on functional groups and their abundance.

	Alcohol	Carboxyl	Ester	Ether	Amide
Alcohol	1201	457 (217*)	129	246	308
Carboxyl		1106	183	156	355
Ester			855	161	101
Ether				1140	53
Amide					602
Net	458	320	454	666	83

* Number of organic compounds with ternary functional groups of “alcohol+carboxyl+amide,” which is the most abundant combination among the ternary groups.

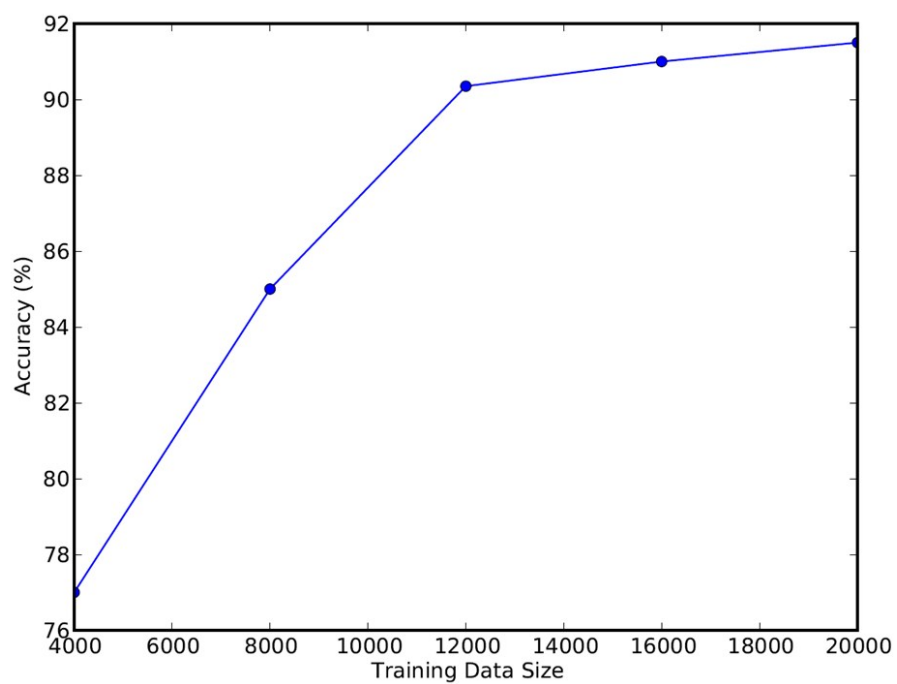


Fig. S1 Accuracy dependence on training data set size, where the accuracy (%) is obtained by the formula (number of test data with error less than 0.5 V)/(total number of test data) \times 100.

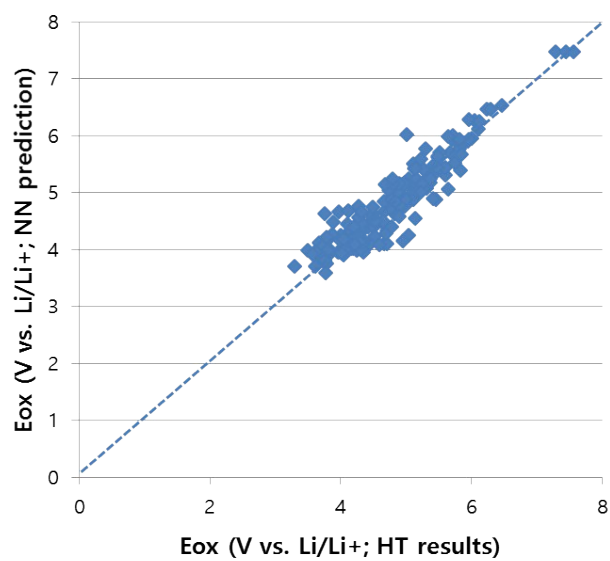


Fig. S2 Comparison of oxidation potentials (E_{ox}) calculated by the quantum chemical method with those predicted by the neural network method in the MAMMBU system.

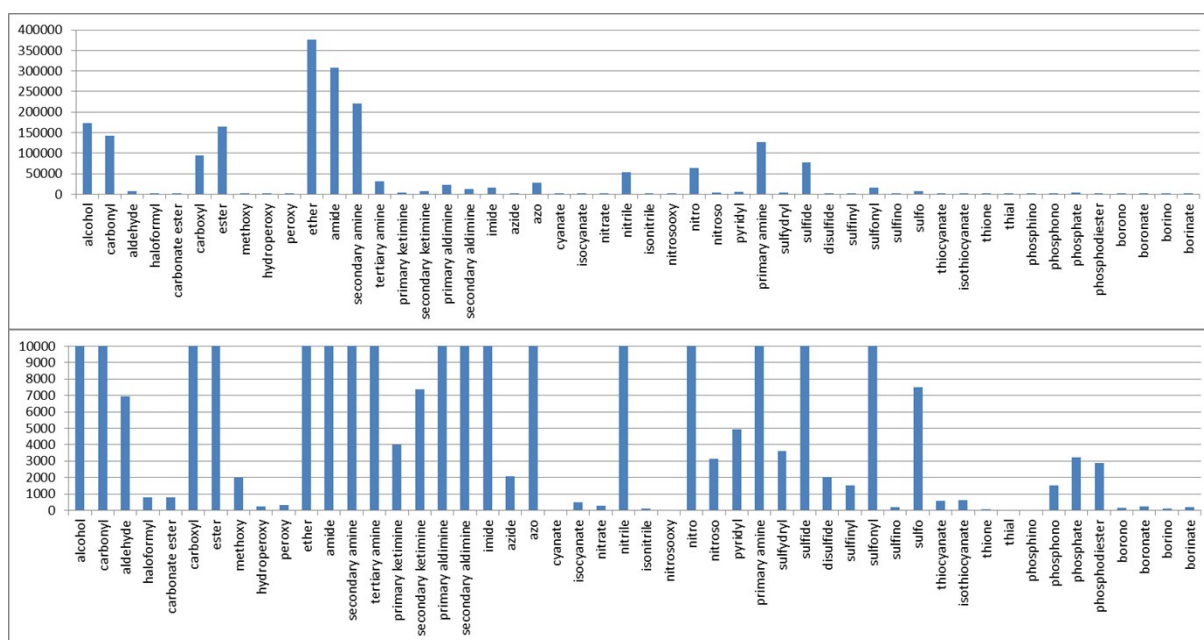


Fig. S3 Classification of 1M organic compounds according to 50 functional groups. (top) the range of ordinate in the graph is between 0 to 400,000, (bottom) the range of ordinate is magnified between 0 to 10,000. Both are same graph and have the same abscissa.