Supporting Information for:

# Liquid electrolyte informatics by exhaustive search with linear regression

Keitaro Sodeyama,*[abc] Yasuhiko Igarashi,[abd] Tomofumi Nakayama,[d] Yoshitaka Tateyama[ace] and Masato Okada[ad]

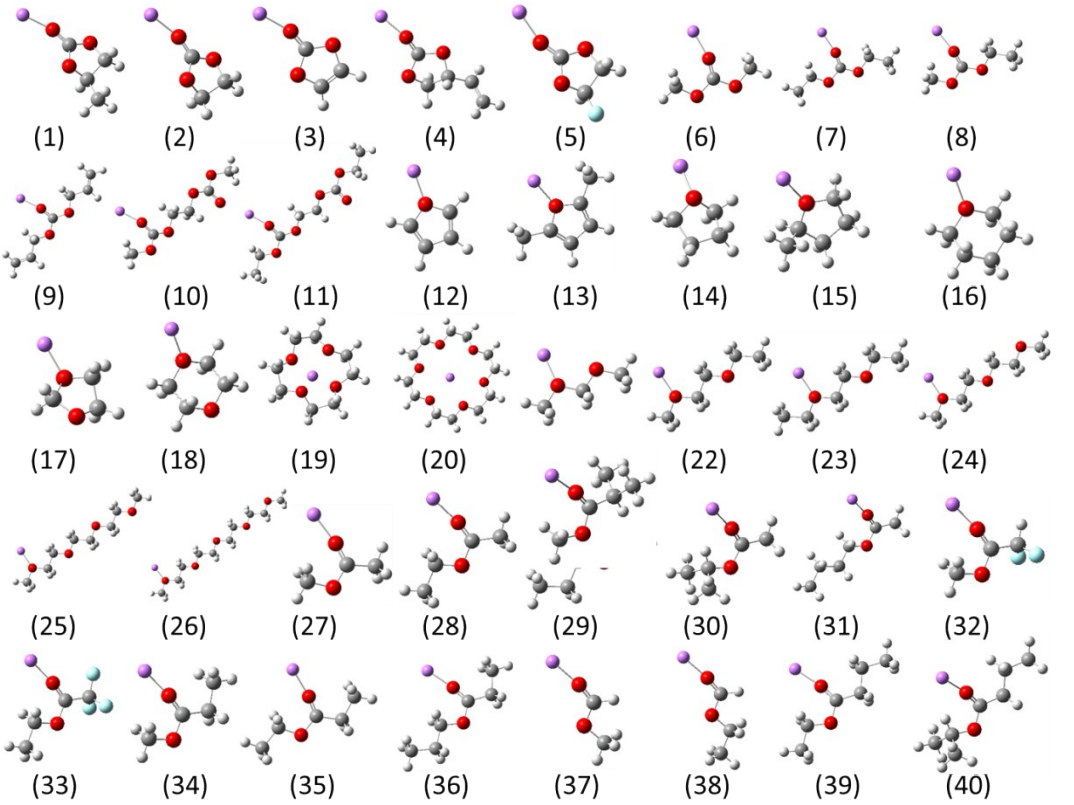
[a] *Center for Materials Research by Information Integration (cMI2), Research and Services Division of Materials Data and Integrated System (MaDIS), National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan.*

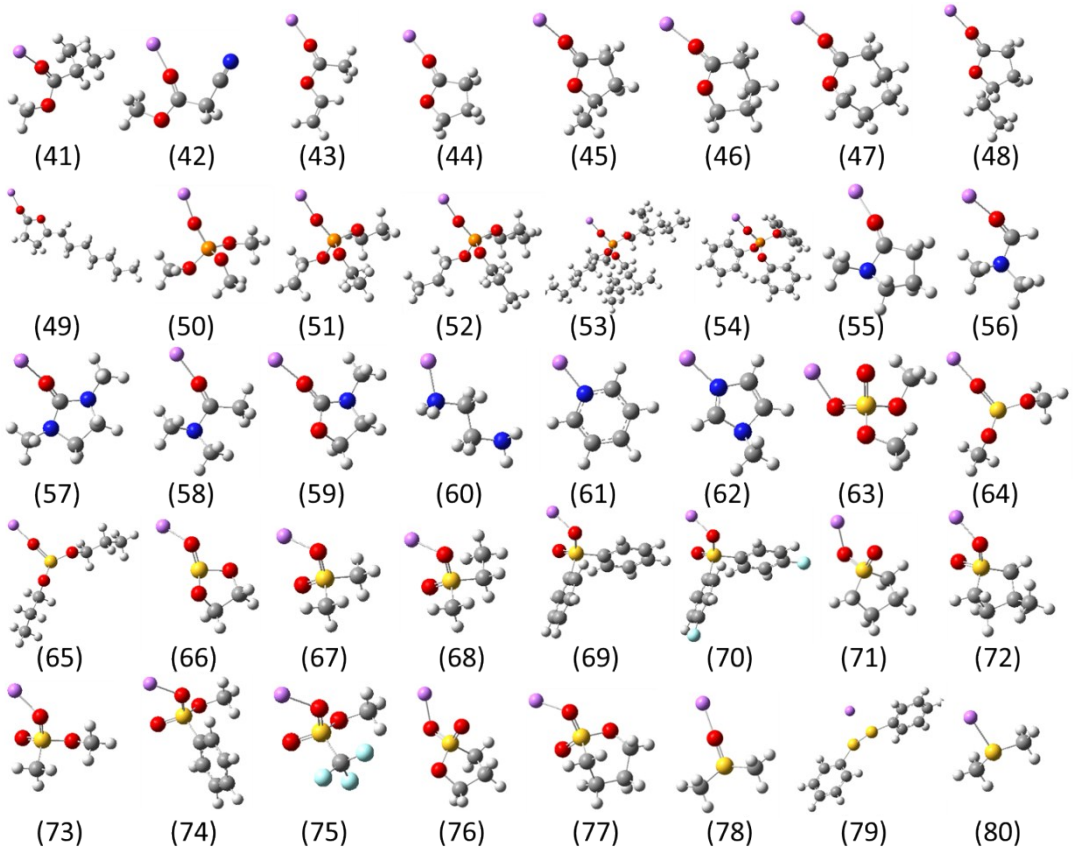
[b] *PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho, Kawaguchi, Saitama 333-0012, Japan.*

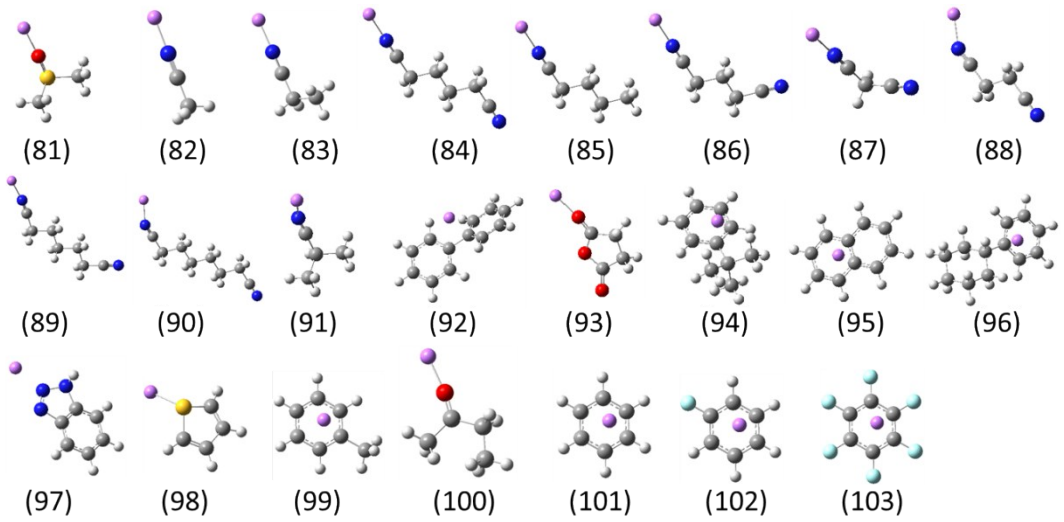
[c] *Elements Strategy Initiative for Catalysts & Batteries (ESICB), Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan.*

[d] *Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5, Kashiwanoha, Kashiwa, Chiba 277-8561, Japan.*

[e] *Center for Green Research on Energy and Environmental Materials (GREEN), and International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan"*


(1)
(2)
(3)
(4)
(5)
(6)
(7)
(8)
(9)
(10)
(11)
(12)
(13)
(14)
(15)
(16)
(17)
(18)
(19)
(20)
(22)
(23)
(24)
(25)
(26)
(27)
(28)
(29)
(30)
(31)
(32)
(33)
(34)
(35)
(36)
(37)
(38)
(39)
(40)


(41)
(42)
(43)
(44)
(45)
(46)
(47)
(48)
(49)
(50)
(51)
(52)
(53)
(54)
(55)
(56)
(57)
(58)
(59)
(60)
(61)
(62)
(63)
(64)
(65)
(66)
(67)
(68)
(69)
(70)
(71)
(72)
(73)
(74)
(75)
(76)
(77)
(78)
(79)
(80)




Scheme S1. 103 solvent molecules for the data-base (Li, purple; O, red; N, blue; C, grey; F, light blue; S, yellow; P, orange; Cl, light blue; H, white).

(1.PC, 2.EC, 3.VC, 4.VEC, 5.FEC, 6.DMC, 7.DEC, 8.EMC, 9.DAC, 10.Dimethyl2,5-dioxahexanedioate, 11.Diethyl 2,5-dioxahexanedioate, 12.Furan, 13.2,5-Dimethyl furane, 14.THF, 15.2-MeTHF, 16.THP, 17.DOL, 18.DIOX, 19.12-Crown 4-ether, 20.18-Crown 6-ether, 21.DMM, 22.DME, 23.DEE, 24.Diglyme, 25.Triglyme, 26.Tetraglyme, 27.MA, 28.EA, 29.PA, 30.iPA, 31.BA, 32.MFA, 33.EFA, 34.MP, 35.EP, 36.PP, 37.MF, 38.EF, 39.EB, 40.iPB, 41.MiB, 42.MCA, 43.VA, 44.GBL, 45.GVL, 46.δ-Valero lactone, 47.ε-Capro lactone, 48.γ-Hexano lactone, 49.γ-Undeca lactone, 50.TMP, 51.TEP, 52.Tri n-propyl phosphate, 53.TOP, 54.TPhP, 55.NMP, 56.DMF, 57.DMI, 58.DMAC, 59.3-Methyl-2-oxazolidinone, 60.Ethylene diamine, 61.Pyridine, 62.N-Methyl imidazole, 63.Dimethyl sulfate, 64.Dimethyl sulfite, 65.Dipropyl sulfite, 66.ES, 67.Dimethyl sulfone, 68.ethylmethyl sulfone, 69.Diphenyl sulfone, 70.Bis(4-Fluoro phenyl sulfone), 71.SL, 72.3-MeSL, 73.Methanesulfonic acid methyl ester, 74.Benzen sulfonic acid methyl ester, 75.Trifluoromethane sulfonic acid methyl ester, 76.PS, 77.BS, 78.DMSO, 79.Diphenly disulfide, 80.Dimethyl sulfide, 81.Diethyl sulfide, 82.AN, 83.PN,84.Adiponitrile, 85.Valeronitrile, 86.Glutaronitrile, 87.Malononitrile, 88.Succinonitrile, 89.Pimelonitrile, 90.Suberonitrile, 91.Isobutyronitrile, 92.Biphenyl, 93.Succinic Anhydride, 94.t-Butyl benzene, 95.Naphthalene, 96.Cyclohexyl benzene, 97.Benzo triazole, 98.Thiophene, 99.Toluene, 100.MEK, 101.Benzene, 102.Fluoro benzene, 103.Hexafluoro benzene).

Table S1(a). Calculated values of 49 solvent molecules for database

| abbreviation | solvent name | $E_{coord}$ (kcal/mol) | HOMO (eV) | LUMO (eV) | Dipole moment (Debye) | Mulliken charge | R(Li-O) (Å) |
|---|---|---|---|---|---|---|---|
| PC | Propylene carbonate | -57.4 | -7.930 | 0.946 | 5.26 | -0.243 | 1.747 |
| EC | Ethylene carbonate | -55.9 | -8.017 | 0.919 | 5.07 | -0.240 | 1.752 |
| VC | Vinylene carbonate | -51.7 | -6.973 | -0.137 | 4.37 | -0.231 | 1.760 |
| VEC | Vinyl ethylene carbonate | -57.6 | -7.829 | -0.720 | 5.28 | -0.240 | 1.746 |
| FEC | Fluoroethylene carbonate | -51.2 | -8.468 | 0.493 | 4.49 | -0.222 | 1.763 |
| DMC | Dimethyl carbonate | -50.0 | -7.774 | 1.115 | 0.34 | -0.306 | 1.747 |
| DEC | Diethyl carbonate | -52.6 | -7.654 | 1.217 | 0.61 | -0.308 | 1.740 |
| EMC | Ethyl methyl carbonate | -51.3 | -7.713 | 1.168 | 0.51 | -0.307 | 1.744 |
| DAC | Diallyl carbonate | -51.9 | -7.419 | -0.238 | 0.49 | -0.306 | 1.740 |
| Dimethyl2,5-dioxahexanedioate | Dimethyl 2,5-dioxahexanedioate | -49.8 | -7.933 | 0.922 | 0.00 | -0.300 | 1.749 |
| Diethyl 2,5-dioxahexanedioate | Diethyl 2,5-dioxahexanedioate | -51.4 | -7.856 | 0.990 | 0.00 | -0.301 | 1.745 |
| Furan | Furan | -31.7 | -6.265 | 0.296 | 0.51 | -0.170 | 1.866 |
| 2,5-Dimethyl furane | 2,5-Dimethyl furane | -36.5 | -5.621 | 0.514 | 0.03 | -0.217 | 1.848 |
| THF | Tetrahydrofuran | -48.7 | -6.832 | 1.380 | 1.43 | -0.323 | 1.808 |
| 2-MeTHF | 2-Methyl tetrahydrofuran | -50.0 | -6.535 | 1.454 | 1.54 | -0.347 | 1.807 |
| THP | Tetrahydropyran | -47.2 | -6.711 | 1.537 | 1.30 | -0.324 | 1.804 |
| DOL | 1,3-Dioxolane | -43.2 | -6.955 | 1.493 | 1.32 | -0.315 | 1.818 |
| DIOX | 1,4-Dioxane | -43.2 | -6.483 | 1.773 | 0.00 | -0.326 | 1.810 |
| 12-Crown 4-ether | 12-Crown 4-ether | -101.1 | -6.655 | 1.965 | 0.00 | -0.331 | 1.889 |
| 18-Crown 6-ether | 18-Crown 6-ether | -104.6 | -6.491 | 1.674 | 0.00 | -0.319 | 2.021 |
| DMM | Dimethoxy methane | -64.4 | -6.846 | 1.459 | 2.17 | -0.298 | 1.905 |
| DME | Dimethoxy ethane | -45.1 | -6.863 | 1.669 | 0.10 | -0.334 | 1.826 |
| DEE | 1,2-Diethoxy ethane | -47.1 | -6.839 | 1.665 | 0.00 | -0.340 | 1.818 |
| Diglyme | Diglyme | -44.7 | -6.898 | 1.616 | 1.13 | -0.334 | 1.827 |
| Triglyme | Triglyme | -44.6 | -6.907 | 1.610 | 0.00 | -0.334 | 1.827 |
| Tetraglyme | Tetraglyme | -44.6 | -6.915 | 1.575 | 1.13 | -0.334 | 1.827 |
| MA | Methyl acetate | -52.0 | -7.371 | 0.339 | 1.73 | -0.265 | 1.755 |
| EA | Ethyl acetate | -53.4 | -7.304 | 0.380 | 1.88 | -0.267 | 1.751 |
| PA | Propyl acetate | -53.8 | -7.299 | 0.385 | 1.94 | -0.266 | 1.750 |
| iPA | Isopropyl acetate | -53.9 | -7.280 | 0.380 | 1.79 | -0.269 | 1.749 |
| BA | Butyl acetate | -54.1 | -7.290 | 0.391 | 1.93 | -0.266 | 1.749 |
| MFA | Methyl difluoroacetate | -55.4 | -8.032 | -0.734 | 1.52 | -0.249 | 1.888 |
| EFA | Ethyl trifluoroacetate | -51.6 | -8.259 | -0.830 | 3.09 | -0.231 | 1.881 |
| MP | Methyl propionate | -52.2 | -7.376 | 0.372 | 1.61 | -0.267 | 1.785 |
| EP | Ethyl propionate | -53.5 | -7.310 | 0.414 | 1.76 | -0.269 | 1.787 |
| PP | Propyl propionate | -53.9 | -7.304 | 0.418 | 1.83 | -0.269 | 1.787 |
| MF | Methyl formate | -52.7 | -7.688 | 0.089 | 3.90 | -0.231 | 1.768 |
| EF | Ethyl formate | -54.2 | -7.603 | 0.105 | 4.00 | -0.234 | 1.763 |
| EB | Ethyl butyrate | -54.3 | -7.303 | 0.414 | 1.68 | -0.270 | 1.795 |
| iPB | Isopropyl butyrate | -55.0 | -7.279 | 0.414 | 1.61 | -0.273 | 1.793 |
| MiB | Methyl Isobutyrate | -53.1 | -7.299 | 0.294 | 1.67 | -0.267 | 1.794 |
| MCA | Methyl cyanoacetate | -58.6 | -8.134 | -0.371 | 5.22 | -0.231 | 1.909 |
| VA | Vinyl acetate | -54.7 | -6.941 | -0.496 | 3.66 | -0.217 | 1.761 |
| GBL | g-Butyro lactone | -56.8 | -7.269 | 0.254 | 4.30 | -0.237 | 1.758 |
| GVL | g-Valero lactone | -58.1 | -7.208 | 0.304 | 4.33 | -0.239 | 1.753 |
| d-Valero lactone | d-Valero lactone | -60.2 | -7.092 | 0.155 | 4.46 | -0.240 | 1.751 |
| e-Capro lactone | e-Capro lactone | -60.2 | -7.074 | 0.288 | 4.45 | -0.239 | 1.753 |
| g-Hexano lactone | g-Hexano lactone | -58.6 | -7.186 | 0.314 | 4.39 | -0.240 | 1.752 |
| g-Undeca lactone | g-Undeca lactone | -59.3 | -7.159 | 0.335 | 4.56 | -0.240 | 1.752 |

Table S1(b). Calculated values of 54 solvent molecules for database

| abbreviation | solvent name | $E_{coord}$ (kcal/mol) | HOMO (eV) | LUMO (eV) | Dipole moment (Debye) | Mulliken charge | R(Li-O) (Å) |
|---|---|---|---|---|---|---|---|
| TMP | Trimethyl phosphate | -65.1 | -7.765 | 1.112 | 3.36 | -0.467 | 1.740 |
| TEP | Triethyl phosphate | -67.7 | -7.650 | 1.130 | 3.43 | -0.470 | 1.733 |
| Tri n-propyl phosphate | Tri n-propyl phosphate | -68.5 | -7.633 | 1.253 | 3.43 | -0.470 | 1.733 |
| TOP | Trioctyl phosphate | -69.2 | -7.622 | 1.103 | 3.39 | -0.473 | 1.730 |
| TPhP | triphenyl phosphate | -68.8 | -6.649 | -0.566 | 3.16 | -0.436 | 1.831 |
| NMP | N-Methyl-2-pyrrolidone | -63.9 | -6.421 | 0.842 | 3.61 | -0.299 | 1.724 |
| DMF | N,N-Dimethyl formamide | -61.2 | -6.623 | 0.731 | 3.70 | -0.297 | 1.736 |
| DMI | 1,3-Dimethyl 2-Imidazolidinone | -64.9 | -6.216 | 1.337 | 3.60 | -0.325 | 1.712 |
| DMAC | N,N-Dimethyl acetamide | -63.3 | -6.411 | 0.800 | 3.55 | -0.301 | 1.723 |
| 3-Methyl-2-oxazolidinone | 3-Methyl-2-oxazolidinone | -62.8 | -6.805 | 1.066 | 4.76 | -0.283 | 1.748 |
| Ethylene diamine | Ethylene diamine | -48.7 | -6.244 | 1.469 | 10.80 | -0.183 | 1.969 |
| Pyridine | Pyridine | -49.4 | -6.985 | -0.796 | 8.72 | -0.223 | 1.941 |
| N-Methyl imidazole | N-Methyl imidazole | -58.3 | -6.135 | 0.640 | 7.99 | -0.238 | 1.912 |
| Dimethyl sulfate | Dimethyl sulfate | -50.2 | -8.195 | 0.341 | 3.40 | -0.392 | 2.029 |
| Dimethyl sulfite | Dimethyl sulfite | -56.7 | -7.416 | -0.327 | 1.41 | -0.456 | 1.901 |
| Dipropyl sulfite | Dipropyl sulfite | -60.8 | -7.292 | -0.248 | 1.55 | -0.456 | 1.901 |
| ES | Ethylene sulfite | -53.0 | -7.725 | -0.823 | 3.12 | -0.423 | 1.758 |
| Dimethyl sulfone | Dimethyl sulfone | -61.0 | -7.683 | 0.905 | 4.47 | -0.460 | 2.023 |
| ethylmethyl sulfone | ethylmethyl sulfone | -62.6 | -7.567 | 0.889 | 4.38 | -0.464 | 2.013 |
| Diphenyl sulfone | Diphenyl sulfone | -66.2 | -7.222 | -1.538 | 5.08 | -0.455 | 2.001 |
| Bis(4-Fluoro phenyl sulfone) | Bis(4-Fluoro phenyl sulfone) | -62.6 | -7.204 | -1.610 | 3.49 | -0.453 | 2.005 |
| SL | Sulfolane | -63.7 | -7.383 | 0.826 | 5.09 | -0.459 | 2.014 |
| 3-MeSL | 3-Methyl sulfolane | -64.3 | -7.366 | 0.737 | 5.09 | -0.461 | 2.012 |
| Methanesulfonic acid methyl ester | Methanesulfonic acid methyl ester | -54.6 | -8.252 | 0.696 | 4.13 | -0.438 | 2.064 |
| Benzen sulfonic acid methyl ester | Benzen sulfonic acid methyl ester | -58.5 | -7.618 | -1.442 | 5.01 | -0.436 | 2.050 |
| Trifluoromethane sulfonic acid methyl ester | Trifluoromethane sulfonic acid methyl ester | -43.4 | -8.981 | 0.016 | 3.21 | -0.408 | 1.812 |
| PS | 1,3-Propane sultone | -57.3 | -7.917 | 0.549 | 5.47 | -0.426 | 2.034 |
| BS | 1,4-Butane sultone | -58.6 | -8.017 | 0.410 | 5.38 | -0.431 | 2.033 |
| DMSO | Dimethyl sulfoxide | -67.8 | -6.010 | 0.963 | 3.82 | -0.542 | 1.718 |
| Diphenly disulfide | Diphenly disulfide | -42.2 | -6.111 | -1.108 | 1.60 | 0.004 | 2.413 |
| Dimethyl sulfide | Dimethyl sulfide | -34.0 | -5.895 | 1.107 | 1.49 | -0.070 | 2.389 |
| Diethyl sulfide | Diethyl sulfide | -37.2 | -5.809 | 0.833 | 1.50 | -0.056 | 2.369 |
| AN | Acetonitrile | -47.0 | -8.933 | 0.898 | 3.74 | -0.181 | 1.920 |
| PN | Propionitrile | -48.4 | -8.802 | 0.587 | 3.83 | -0.185 | 1.914 |
| Adiponitrile | Adiponitrile | -45.3 | -8.976 | 0.312 | 0.00 | -0.176 | 1.916 |
| Valeronitrile | Valeronitrile | -49.7 | -8.704 | 0.728 | 4.06 | -0.183 | 1.908 |
| Glutaronitrile | Glutaronitrile | -44.2 | -9.081 | -0.136 | 3.72 | -0.170 | 1.921 |
| Malononitrile | Malononitrile | -38.5 | -9.544 | -0.510 | 3.62 | -0.153 | 1.945 |
| Succinonitrile | Succinonitrile | -41.1 | -9.310 | -0.097 | 0.00 | -0.165 | 1.929 |
| Pimelonitrile | Pimelonitrile | -46.7 | -8.858 | 0.346 | 3.73 | -0.177 | 1.914 |
| Suberonitrile | Suberonitrile | -47.3 | -8.789 | 0.497 | 0.00 | -0.180 | 1.912 |
| Isobutyronitrile | Isobutyronitrile | -49.5 | -8.727 | 0.642 | 3.85 | -0.189 | 1.973 |
| Biphenyl | Biphenyl | -38.0 | -6.236 | -0.917 | 0.00 | 0.034 | 2.230 |
| Succinic Anhydride | Succinic Anhydride | -48.1 | -7.794 | -0.866 | 4.23 | -0.199 | 1.784 |
| t-Butyl benzene | t-Butyl benzene | -44.0 | -6.580 | -0.142 | 0.36 | 0.100 | 2.360 |
| Naphthalene | Naphthalene | -41.7 | -5.977 | -1.197 | 0.00 | 0.017 | 2.336 |
| Cyclohexyl benzene | Cyclohexyl benzene | -44.6 | -6.543 | -0.132 | 0.43 | 0.064 | 2.352 |
| Benzo triazole | Benzo triazole | -56.8 | -6.694 | -1.325 | 3.79 | -0.058 | 2.022 |
| Thiophene | Thiophene | -36.7 | -6.474 | -0.408 | 0.47 | 0.139 | 2.518 |
| Toluene | Toluene | -41.9 | -6.571 | -0.125 | 0.38 | 0.041 | 2.324 |
| MEK | Methyl ethyl ketone | -53.0 | -6.601 | -0.386 | 2.77 | -0.225 | 1.759 |
| Benzene | Benzene | -39.1 | -6.893 | -0.177 | 0.00 | 0.032 | 2.355 |
| Fluoro benzene | Fluoro benzene | -34.0 | -6.805 | -0.499 | 1.35 | 0.012 | 2.409 |
| Hexafluoro benzene | Hexafluoro benzene | -11.7 | -7.483 | -1.005 | 0.00 | 0.142 | 2.532 |

Table S2. Estimated and first-principles calculation values of coordination energies of solvents (kcal/mol)

| | TRUE | MLR | LASSO | ES-LR | | TRUE | MLR | LASSO | ES-LR |
|---|---|---|---|---|---|---|---|---|---|
| PC | -57.4 | -52.7 | -52.1 | -55.1 | TMP | -65.1 | -58.8 | -64.7 | -64.6 |
| EC | -55.9 | -57.1 | -50.6 | -55.8 | TEP | -67.6 | -57.8 | -64.0 | -64.6 |
| VC | -51.8 | -51.8 | -51.1 | -53.4 | TOP | -69.2 | -116.9 | -65.2 | -70.8 |
| FEC | -51.1 | -49.3 | -49.6 | -52.6 | NMP | -63.9 | -56.9 | -55.5 | -59.2 |
| DMC | -50.0 | -54.7 | -55.7 | -53.3 | DMF | -61.2 | -56.2 | -55.5 | -58.2 |
| DEC | -52.6 | -52.1 | -55.2 | -53.7 | DMI | -64.9 | -55.4 | -57.9 | -61.3 |
| EMC | -51.3 | -52.9 | -55.7 | -53.8 | DMAC | -63.3 | -58.2 | -56.2 | -59.7 |
| Furan | -31.8 | -40.3 | -49.5 | -48.1 | Ethylene diamine | -48.7 | -53.6 | -49.6 | -49.6 |
| 2,5-Dimethyl furane | -36.5 | -52.3 | -52.6 | -54.0 | Pyridine | -49.3 | -45.7 | -51.9 | -50.5 |
| THF | -48.8 | -54.0 | -57.0 | -53.7 | N-Methyl imidazole | -58.4 | -63.4 | -52.2 | -56.0 |
| 2-MeTHF | -49.9 | -52.5 | -56.9 | -54.7 | Dimethyl sulfate | -50.2 | -49.0 | -59.7 | -55.7 |
| THP | -47.2 | -51.0 | -56.4 | -53.0 | SL | -63.8 | -54.5 | -62.0 | -59.4 |
| DOL | -43.2 | -61.3 | -57.5 | -55.2 | Methanesulfonic acid methyl ester | -54.7 | -47.6 | -50.8 | -50.2 |
| DIOX | -43.2 | -54.0 | -57.2 | -54.0 | Benzen sulfonic acid methyl ester | -58.5 | -186.1 | -64.3 | -63.3 |
| 12-Crown 4-ether | -101.2 | -68.6 | -56.4 | -57.9 | PS | -57.4 | -63.3 | -62.8 | -61.9 |
| 18-Crown 6-ether | -104.5 | -58.5 | -55.4 | -54.8 | BS | -58.5 | -62.6 | -61.9 | -60.7 |
| DMM | -64.4 | -51.3 | -53.4 | -49.1 | DMSO | -67.8 | -63.9 | -68.1 | -67.6 |
| DME | -45.1 | -55.3 | -57.5 | -54.3 | Diphenly disulfide | -42.2 | -38.2 | -39.1 | -44.6 |
| DEE | -47.1 | -57.5 | -57.6 | -56.5 | Dimethyl sulfide | -33.9 | -32.6 | -38.3 | -32.7 |
| Diglyme | -44.7 | -56.9 | -58.0 | -57.6 | Diethyl sulfide | -37.2 | -36.8 | -42.9 | -39.3 |
| Triglyme | -44.6 | -60.2 | -57.7 | -60.3 | AN | -47.0 | -48.9 | -46.5 | -42.5 |
| Tetraglyme | -44.6 | -61.4 | -57.4 | -62.2 | PN | -48.4 | -44.2 | -45.0 | -43.9 |
| MA | -52.0 | -48.9 | -52.3 | -50.3 | Adiponitrile | -45.3 | -38.8 | -46.6 | -48.4 |
| EA | -53.4 | -49.9 | -52.3 | -50.3 | Valeronitrile | -49.7 | -45.6 | -45.7 | -46.6 |
| PA | -53.8 | -50.1 | -52.7 | -51.6 | Glutaronitrile | -44.2 | -44.9 | -47.1 | -48.9 |
| iPA | -53.9 | -52.0 | -53.3 | -52.5 | Malononitrile | -38.5 | -52.6 | -45.4 | -47.5 |
| MP | -52.2 | -51.1 | -52.5 | -50.8 | Succinonitrile | -41.0 | -53.6 | -46.4 | -50.6 |
| EP | -53.5 | -51.7 | -52.6 | -51.2 | Suberonitrile | -47.3 | -72.4 | -47.5 | -52.8 |
| PP | -53.9 | -51.9 | -52.8 | -51.2 | Isobutyronitrile | -49.5 | -46.5 | -47.1 | -43.0 |
| MF | -52.7 | -46.6 | -50.3 | -46.8 | Biphenyl | -38.0 | -40.0 | -37.4 | -42.4 |
| EF | -54.2 | -49.5 | -50.6 | -48.0 | Succinic Anhydride | -48.1 | -55.7 | -49.7 | -55.6 |
| EB | -54.3 | -51.0 | -53.2 | -52.1 | t-Butyl benzene | -44.0 | -29.8 | -30.8 | -31.4 |
| MiB | -53.2 | -51.3 | -52.6 | -50.9 | Naphthalene | -41.7 | -36.6 | -36.7 | -39.3 |
| MCA | -58.6 | -52.8 | -50.8 | -52.3 | Toluene | -41.9 | -30.2 | -35.7 | -33.8 |
| VA | -54.7 | -55.9 | -64.2 | -61.1 | MEK | -53.0 | -50.0 | -49.6 | -50.2 |
| GBL | -56.8 | -52.3 | -51.3 | -54.7 | Benzene | -39.2 | -35.8 | -35.8 | -33.0 |
| GVL | -58.1 | -52.5 | -51.0 | -54.3 | Fluoro benzene | -33.9 | -39.4 | -43.7 | -36.7 |
| d-Valero lactone | -60.2 | -52.7 | -51.8 | -56.3 | Hexafluoro benzene | -11.7 | -38.6 | -38.3 | -27.9 |
| e-Capro lactone | -60.2 | -53.6 | -51.1 | -55.0 | | | | | |
| g-Hexano lactone | -58.6 | -52.7 | -51.0 | -54.3 | | | | | |

Figure S1. Bar graph of absolute value of coefficients about coordination energy prediction with MLR, LASSO, and ES-LiR.

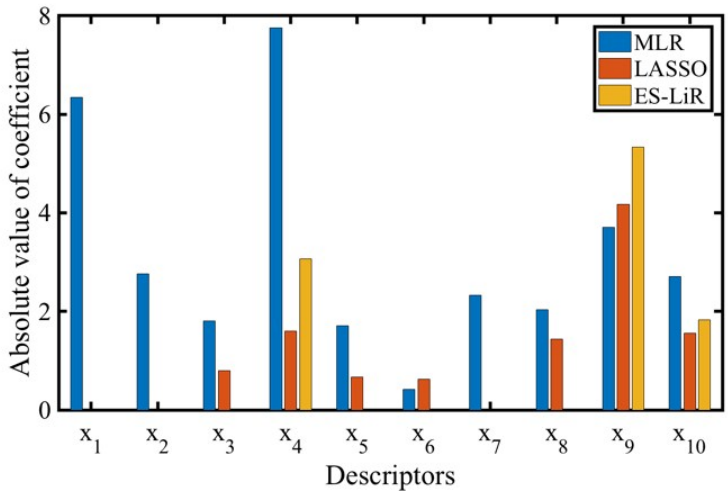


Figure S2. All indicator weight diagram for coordination energy prediction.

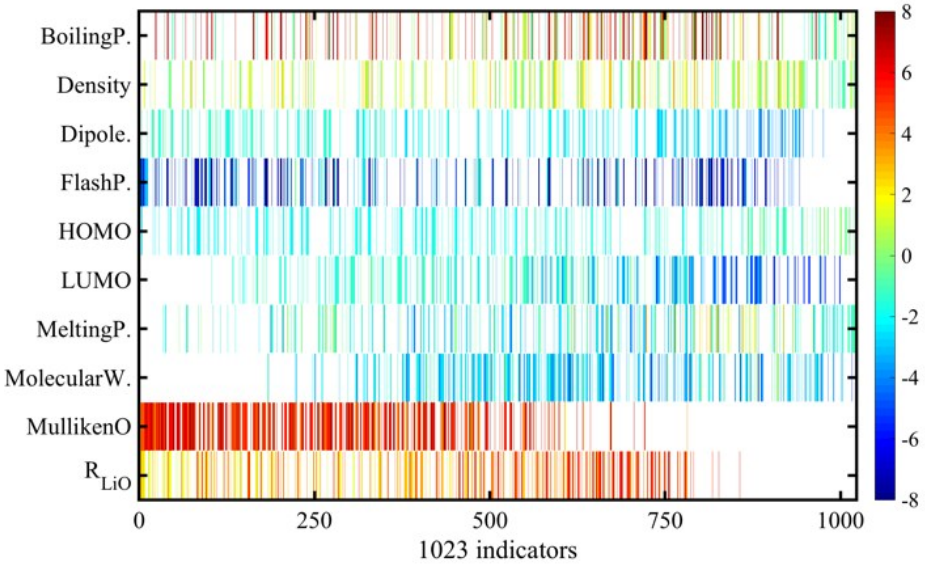


Figure S3. All indicator weight diagram for melting point prediction.