

## Supplementary Information

### **Design of novel additives and nonaqueous solvents for lithium-ion batteries through screening of cyclic organic molecules: an *ab initio* study of redox potentials**

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Table S1. E<sub>ox</sub> values for 142 cyclic organic molecules

| Compounds               | E <sub>ox</sub> | Compounds             | E <sub>ox</sub> | Compounds                     | E <sub>ox</sub> | Compounds                        | E <sub>ox</sub> |
|-------------------------|-----------------|-----------------------|-----------------|-------------------------------|-----------------|----------------------------------|-----------------|
| 4H-Quinolizine          | 2.54            | Imidazolidine         | 3.95            | 2,1-Benzisoxazole             | 4.56            | Tetrahydrofuran                  | 5.22            |
| Azepine                 | 2.73            | 2H-1-Benzopyran       | 3.98            | 1H-Imidazole                  | 4.6             | Quinoxaline                      | 5.22            |
| 4H-1,4-Oxazine          | 2.78            | Piperidine            | 3.99            | Furan                         | 4.62            | Benzene                          | 5.23            |
| 4H-1,4-Benzoxazine      | 3.01            | Indole                | 3.99            | Benzimidazole                 | 4.62            | Norpinane(bicyclo[3,1,1]heptane) | 5.24            |
| 2H-1,2-Oxazine          | 3.02            | Morpholine            | 4.03            | 6H-1,2-Oxazine                | 4.64            | 1,3,5-Oxadiazine                 | 5.25            |
| 5H-1,2,5-Oxathiazole    | 3.16            | Thiomorpholine        | 4.04            | 1H-2-Benzopyran-1-one         | 4.65            | 2H-Pyrrole                       | 5.26            |
| 2-Pyrroline             | 3.21            | Carbazole             | 4.04            | 2-Thiazoline                  | 4.66            | Pyrazine                         | 5.26            |
| Pyrazolidine            | 3.22            | 3H-1,2-Oxathiole      | 4.05            | Isoquinoline                  | 4.66            | Pyridine                         | 5.28            |
| Phenothiazine           | 3.28            | Pyrrole               | 4.13            | Phenazine                     | 4.66            | 1,2,3-Triazine                   | 5.28            |
| Phenoxazine             | 3.29            | 1,2,6-Oxathiazine     | 4.13            | Thiophene                     | 4.68            | 1,2,4-Dioxazole                  | 5.31            |
| Cyclopenta[b]pyridine   | 3.32            | 3H-2-Benzopyran-3-one | 4.15            | 1,2,3,4-Tetrahydronaphthalene | 4.71            | Adamantane                       | 5.35            |
| 1,2,4-Oxadiazine        | 3.36            | 2-Imidazoline         | 4.17            | Cinnoline                     | 4.72            | Pyrimidine                       | 5.36            |
| Indoline                | 3.45            | 2H-1,4-Oxazine        | 4.19            | 3H-Indole                     | 4.73            | Pteridine                        | 5.37            |
| 2H-Indene               | 3.47            | 2H-1,4-Benzoxazine    | 4.19            | 1H-2,3-Benzoxazine            | 4.75            | Decahydronaphthalene             | 5.39            |
| 2H-1,3-Dithiole         | 3.56            | Coumaran              | 4.21            | Quinoline                     | 4.8             | 1,3-Dioxolane                    | 5.41            |
| Piperazine              | 3.57            | Xanthene              | 4.23            | Pyridazine                    | 4.82            | Isothiazole                      | 5.41            |
| Thiepin                 | 3.63            | Acridine              | 4.28            | Phthalazine                   | 4.83            | 1,8-Naphthyridine                | 5.41            |
| 1,3-Oxathiole           | 3.65            | Indene                | 4.29            | 3H-Pyrrole                    | 4.84            | Cyclopropane                     | 5.42            |
| Oxepin                  | 3.65            | Phenanthrene          | 4.3             | Benzothiazole                 | 4.88            | Cyclobutane                      | 5.44            |
| 1,2-Dioxin              | 3.68            | Fluorene              | 4.32            | 2H-1,3,4-Dioxazole            | 4.92            | 4H-Pyran-4-One                   | 5.46            |
| 3H-1,2-Dithiole         | 3.7             | Tetrahydrothiophene   | 4.34            | 1,2,3,5-Oxatriazole           | 4.96            | 1,2,3-Triazole                   | 5.56            |
| 2H-Pyran                | 3.72            | Benzo(b)thiophene     | 4.35            | 2H-Pyran-2-One                | 4.96            | Isoxazole                        | 5.65            |
| Azulene                 | 3.73            | Naphthalene           | 4.36            | 2H-1-Benzopyran-2-one         | 4.96            | Norbornane                       | 5.65            |
| 2H-1,2,4-Benzoxadiazine | 3.73            | Pyrano[3,4-b]pyrrole  | 4.39            | 1,2,4-Triazine                | 4.98            | 1,2,4-Triazole                   | 5.7             |
| Phenylene               | 3.78            | 2H-1,3-Oxazine        | 4.41            | 1,4-Dioxane                   | 4.99            | 1,2,3,4-Oxatriazole              | 5.74            |
| Isobenzofuran           | 3.8             | 6H-1,3-Oxazine        | 4.41            | Benzoxazole                   | 4.99            | Cyclohexane                      | 5.76            |
| Anthracene              | 3.81            | 2H-1,3-Benzoxazine    | 4.41            | 1H-Isoindole                  | 5.05            | 1,3,4-Thiadiazole                | 5.84            |
| 3H-1,2,3-Dioxazole      | 3.83            | 1,3,5-Trithiane       | 4.44            | Thiazole                      | 5.07            | 1,3,5-Triazine                   | 5.87            |
| Benzo(c)thiophene       | 3.83            | 4H-3,1-Benzoxazine    | 4.45            | Quinazoline                   | 5.08            | 2H-Imidazole                     | 5.94            |
| Pyrrolidine             | 3.84            | 4H-1,2-Oxazine        | 4.47            | 4H-1-Benzopyran-4-one         | 5.09            | Cyclopentane                     | 6.12            |
| 2-Pyrazoline            | 3.86            | Benzofuran            | 4.47            | Pyrazole                      | 5.11            | 5-Oxazolone                      | 6.13            |
| 3-Pyrroline             | 3.88            | 1,4-Dithiane          | 4.48            | Benzisoxazole                 | 5.11            | 1,3,4-Oxadiazole                 | 6.31            |
| Quinuclidine            | 3.88            | 1,3-Dioxin            | 4.51            | 1,7-Naphthyridine             | 5.11            | 1,2,4-Oxadiazole                 | 6.58            |
| Imidazoline-2-thione    | 3.89            | 1H-Indazole           | 4.51            | 1,6-Naphthyridine             | 5.14            | 1,2,5-Oxadiazole                 | 6.93            |
| 1,3,2-Dioxazole         | 3.9             | 4H-1,2-Diazepine      | 4.52            | Oxazole                       | 5.2             |                                  |                 |
| 1,2,5-Oxathiazine       | 3.94            | 1,2,3-Oxadiazole      | 4.54            | 1,5-Naphthyridine             | 5.21            |                                  |                 |

Table S2.  $E_{rd}$  for 142 cyclic organic molecules

| Compounds                        | $E_{rd}$ | Compounds            | $E_{rd}$ | Compounds             | $E_{rd}$ | Compounds               | $E_{rd}$ |
|----------------------------------|----------|----------------------|----------|-----------------------|----------|-------------------------|----------|
| Cyclopropane                     | -1.65    | Xanthene             | -0.23    | Benzothiazole         | 0.44     | 2,1-Benzisoxazole       | 1.05     |
| Cyclobutane                      | -1.46    | Thiophene            | -0.2     | 1H-Isoindole          | 0.53     | 2H-Pyran-2-One          | 1.07     |
| 1,4-Dioxane                      | -1.38    | Imidazoline-2-thione | -0.2     | 1,2,4-Oxadiazole      | 0.54     | Thiepin                 | 1.1      |
| Decahydronaphthalene             | -1.38    | Phenothiazine        | -0.1     | Phenalene             | 0.54     | 1,6-Naphthyridine       | 1.1      |
| Cyclopentane                     | -1.37    | Benzimidazole        | -0.09    | Cyclopenta[b]pyridine | 0.55     | 1,7-Naphthyridine       | 1.12     |
| Cyclohexane                      | -1.35    | Oxazole              | -0.07    | Isobenzofuran         | 0.56     | 1,8-Naphthyridine       | 1.13     |
| 1,3-Dioxolane                    | -1.34    | Benzofuran           | -0.03    | 5-Oxazolone           | 0.6      | 1,5-Naphthyridine       | 1.13     |
| Piperazine                       | -1.28    | 2H-1,3-Dithiole      | -0.02    | Pyrimidine            | 0.62     | Quinazoline             | 1.14     |
| Tetrahydrofuran                  | -1.24    | Indene               | 0        | Benzisoxazole         | 0.64     | 1,2,3,4-Oxatriazole     | 1.15     |
| Morpholine                       | -1.24    | 1,2,3-Triazole       | 0.02     | 4H-Pyran-4-One        | 0.66     | 2H-1-Benzopyran-2-one   | 1.23     |
| Quinuclidine                     | -1.23    | 2-Thiazoline         | 0.04     | 1,3,5-Trithiane       | 0.66     | Azulene                 | 1.29     |
| Norpinane(bicyclo[3,1,1]heptane) | -1.2     | Benzo(b)thiophene    | 0.07     | 2H-1,4-Oxazine        | 0.67     | 1,2,3-Triazine          | 1.33     |
| Norbornane                       | -1.19    | Isoxazole            | 0.1      | Benzo(c)thiophene     | 0.68     | Acridine                | 1.33     |
| Pyrrole                          | -1.16    | 1,3,4-Oxadiazole     | 0.1      | Isoquinoline          | 0.74     | Quinoxaline             | 1.35     |
| Piperidine                       | -1.15    | Thiomorpholine       | 0.1      | 2H-1,3-Oxazine        | 0.78     | Cinnoline               | 1.36     |
| 2-Pyrroline                      | -1.14    | 2H-1,3,4-Dioxazole   | 0.13     | 2H-1,4-Benzoxazine    | 0.79     | 4H-1,2-Diazepine        | 1.4      |
| Pyrrolidine                      | -1.12    | Carbazole            | 0.17     | Quinoline             | 0.8      | 1,2,4-Triazine          | 1.52     |
| Pyrazolidine                     | -1.08    | Fluorene             | 0.19     | 1,2,3-Oxadiazole      | 0.84     | 1,2,3,5-Oxatriazole     | 1.65     |
| 1H-Imidazole                     | -1.02    | 2H-Pyran             | 0.2      | 1,3-Oxathiole         | 0.84     | 3H-2-Benzopyran-3-one   | 1.65     |
| Adamantane                       | -1.01    | Thiazole             | 0.21     | 1,3,5-Triazine        | 0.85     | Phenazine               | 1.8      |
| 3-Pyrroline                      | -0.71    | Pyridine             | 0.21     | 1H-2,3-Benzoxazine    | 0.86     | 3H-1,2-Dithiole         | 1.91     |
| Imidazolidine                    | -0.71    | 1H-Indazole          | 0.23     | Pyridazine            | 0.87     | Pteridine               | 1.93     |
| 2-Imidazoline                    | -0.56    | 2H-1-Benzopyran      | 0.32     | Azepine               | 0.87     | 3H-1,2,3-Dioxazole      | 2.04     |
| Furan                            | -0.5     | Tetrahydrothiophene  | 0.33     | Oxepin                | 0.87     | 3H-1,2-Oxathiole        | 2.24     |
| Pyrazole                         | -0.5     | Isothiazole          | 0.33     | 2H-1,3-Benzoxazine    | 0.9      | 4H-1,2-Oxazine          | 2.41     |
| 1,2,3,4-Tetrahydronaphthalene    | -0.5     | Benzoxazole          | 0.33     | Pyrazine              | 0.93     | 1,2,6-Oxathiazine       | 2.58     |
| 1,3-Dioxin                       | -0.49    | 3H-Pyrrole           | 0.35     | 1H-2-Benzopyran-1-one | 0.93     | 1,3,2-Dioxazole         | 3.01     |
| Indoline                         | -0.47    | Naphthalene          | 0.39     | 6H-1,2-Oxazine        | 0.94     | 2H-1,2,4-Benzoxadiazine | 3.33     |
| 4H-1,4-Benzoxazine               | -0.47    | 4H-Quinolizine       | 0.39     | Phthalazine           | 0.94     | 2H-1,2-Oxazine          | 3.48     |
| Benzene                          | -0.41    | 1,3,4-Thiadiazole    | 0.4      | Anthracene            | 0.96     | 1,2,5-Oxathiazine       | 3.51     |
| 4H-1,4-Oxazine                   | -0.39    | 6H-1,3-Oxazine       | 0.4      | 1,2,5-Oxadiazole      | 0.97     | 5H-1,2,5-Oxathiazole    | 3.56     |
| Phenoxazine                      | -0.36    | Phenanthrene         | 0.4      | 2H-Indene             | 0.97     | 1,2,4-Dioxazole         | 3.71     |
| Coumaran                         | -0.35    | 4H-3,1-Benzoxazine   | 0.42     | 1,3,5-Oxadiazine      | 0.99     | 1,2,4-Oxadiazine        | 4.11     |
| Indole                           | -0.31    | 2H-Pyrrole           | 0.43     | Pyrano[3,4-b]pyrrole  | 1.01     | 1,2-Dioxin              | 5.44     |
| 2-Pyrazoline                     | -0.27    | 1,4-Dithiane         | 0.43     | 4H-1-Benzopyran-4-one | 1.01     |                         |          |
| 1,2,4-Triazole                   | -0.25    | 3H-Indole            | 0.43     | 2H-Imidazole          | 1.05     |                         |          |