## Supplementary Table 1 for: Quantum chemical calculations of lithium-ion battery electrolyte and interphase species

| Molecule Number | Structure                                      | Fragmentation Steps |
|-----------------|--|---------------------|
|                 | OLi <sup>+</sup>                               |                     |
|                 | 0 10   |                     |
| 1               |  | MAX                 |
|                 | 0.<br>// `,Li+                                 |                     |
| 2               | Ó  | MAX                 |
|                 | O-ri+  |                     |
| 3               | 000  | MAX                 |
|                 | 0~~Li+   |                     |
| 4               | 0 0  | MAX                 |
|                 | O-Li <sup>+</sup>                              |                     |
| 5               | $\bigcirc \bigcirc \bigcirc \bigcirc \bigcirc$ | MAX                 |
|                 | 0Li+   |                     |
| 6               | 7 0 0  | MAX                 |
|                 | Q−Li <sup>+</sup>                              |                     |
| 7               | 000  | MAX                 |
|                 | 0Li+   |                     |
| 8               | 0 0  | MAX                 |
|                 | +Li, O   |                     |
| 9               | 0 0  | MAX                 |
| θ               | ·  | IVIAA               |

|    | ٥Li+  |       |
|----|---|-------|
|    | 0   |       |
| 10 | F   | MAX   |
|    | OLi+  |       |
|    | 0 0   |       |
| 11 | F   | MAX   |
| 11 | 0,  | WAX   |
|    | 0 Li+                                       |       |
| 12 | F ~   | MAX   |
|    | ,   |       |
|    | 0   |       |
| 13 | F   | MAX   |
|    | F. J. F                                     |       |
| 14 | Ll'F*'  <b>*</b> F<br>F                     | MAX   |
|    | O S N S O CF <sub>3</sub> U CF <sub>3</sub> |       |
| 15 | Lit   | MAX   |
| 10 | 0 <sub>2</sub> N <sub>2</sub> 0             | WAA   |
|    | O S N S O F O O O                           |       |
| 16 | Li*   | MAX   |
|    | Li+-O-, Li+                                 | 24137 |
| 17 | 0 0   | MAX   |
| 18 | O- OH                                       | MAX   |
| 10 | 0   |       |
| 19 | но он                                       | MAX   |
|    | O- O.<br>+Li´_)// Li+                       |       |
| 20 | 0 0   | MAX   |

|    | 1:+  |          |
|----|--|----------|
|    | O, ,O  |          |
|    |  |          |
| 21 | U, O   | MAX      |
| 21 | HO, O,   | WAX      |
| 20 | ) Li <sup>+</sup>                                | 3.6.4.37 |
| 22 | HQ ,Q  | MAX      |
|    | <b>—</b>   |          |
| 23 | O OH   | MAX      |
| 24 | Li~ <sup>OH</sup>                                | MAX      |
| 25 | Li-OH  | MAX      |
| 26 | Li~F   | MAX      |
| 27 | O <sub>2</sub>                                   | MAX      |
| 28 | H <sub>2</sub>                                   | MAX      |
| 29 | F <sub>2</sub>                                   | MAX      |
| 30 | O=C=O  | MAX      |
| 31 |  | MAX      |
|    | F <sub>C</sub> CH <sub>3</sub><br>H <sub>2</sub> |          |
| 32 |  | MAX      |
| 33 | _0_  | MAX      |
| 34 | H <sub>3</sub> O                                 | MAX      |
| 35 | HF   | MAX      |
|    | Li <sup>+</sup> 0                                |          |
|    | 0 0 Li+  | 3.64.77  |
| 36 |  | MAX      |
|    | Li <sup>+</sup> O O OH                           |          |
| 37 |  | MAX      |
|    | O  | 2.22.22  |
|    | HO O OH OH                                       |          |
| 38 | Ö  | MAX      |
|    | O F  |          |
|    | 000  |          |
| 39 | 0,   | MAX      |

|     | 0                                       |              |
|-----|---|--------------|
|     | Li+ 1                                   |              |
|     |   |              |
| 40  | Öʻ-Li <sup>+</sup>                      | 3            |
|     | Li+~0                                   |              |
|     | O OH                                    |              |
|     | 0, 0, 0                                 |              |
| 41  | O                                       | 3            |
|     | O                                       |              |
|     | HO O OH                                 |              |
| 40  |   | 9            |
| 42  | о г                                     | 3            |
|     | Li <sup>+-</sup> O F                    |              |
|     | 000                                     |              |
| 43  | Oʻ-Li <sup>+</sup>                      | 2            |
| 10  | 0                                       |              |
|     |   |              |
|     | 0, 0,                                   |              |
| 44  | F O <sup>Ll</sup>                       | 2            |
|     | Li+ O F                                 |              |
|     |   |              |
|     |   |              |
| 45  | F 0.74                                  | 2            |
|     | Li <sup>+</sup> -O F F                  |              |
|     | $\frac{1}{2}$                           |              |
| 4.0 | O Li <sup>+</sup>                       | 9            |
| 46  |   | 2            |
|     | Li+ O F                                 |              |
|     | 000                                     |              |
| 47  | ϝ Ω΄- <sup>Li+</sup>                    | 2            |
|     | 0                                       |              |
|     | Li <sup>+</sup>   O O - Li <sup>+</sup> |              |
| 48  | 0 0 0-6                                 | MAX          |
|     | =0. <sub>Li</sub> +                     |              |
|     | O. Li+<br>O. Li+                        |              |
| 49  |   | MAX          |
|     | , ;+·0                                  |              |
|     | Li+-O<br>O OH                           |              |
| 50  | 0, 0, 0                                 | MAX          |
|     | 0                                       |              |
| F-1 | HO O O-Li <sup>+</sup>                  | D. C. A. 3.7 |
| 51  | 110 0                                   | MAX          |

|          | 0                                     |           |
|----------|---------------------------------------|-----------|
|          | но                                    |           |
|          | Lit                                   | 3.64.77   |
| 52       | 0                                     | MAX       |
| <b>.</b> | но                                    | 3.6437    |
| 53       |                                       | MAX       |
|          | Li <sup>+</sup> O OH                  |           |
| 54       | F F                                   | MAX       |
|          | Li <sup>+</sup> O F                   |           |
| 55       | O O O O O O O O O O O O O O O O O O O | MAX       |
|          | Li+ O                                 |           |
| 56       | 0 0 F                                 | MAX       |
|          | Li <sup>+</sup> O F O-Li <sup>+</sup> |           |
| 57       | 0 0 0                                 | MAX       |
|          | Li <sup>+</sup> 0                     |           |
|          | 0, 0, \(\frac{1}{2}\)                 |           |
| 58       | F                                     | MAX       |
|          | O FLi+                                |           |
| 59       | 0, 0,                                 | MAX       |
|          | Li+ 0                                 |           |
| 60       | 0´ 0´ \Li+                            | N. ( A 37 |
| 60       | ı lit                                 | MAX       |
| 61       | ∕^o <sup>Li⁺</sup>                    | MAX       |
| 62       | ОН                                    | MAX       |
| 63       | +LiOOLi+                              | MAX       |
|          | 0 0                                   |           |
| 64       | Li <sup>+</sup>                       | MAX       |
| 04       | +  i                                  | MAA       |
|          | , jo                                  |           |
|          | 0 F                                   |           |
| 65       | LI <sup>T</sup>                       | MAX       |

|    | *Li`.`0 \\^0`Li*                            |     |
|----|---|-----|
| 66 | F F   | MAX |
|    | o <b>↑</b> F                                |     |
| 67 | Ľi <sup>‡</sup> . O´ ´ Ĺi <sup>†</sup>      | MAX |
| 68 | HO^^_Li+                                    | MAX |
|    | HO  |     |
| 69 | LI OH                                       | MAX |
| 70 | HO ~  | MAX |
| 71 | *Li``0^\\_0`Li*                             | MAX |
| 72 | HO Li+                                      | MAX |
| 73 | HO  | MAX |
|    | +LiO  |     |
| 74 | 0 0 1                                       | MAX |
|    | +Li, Li+                                    |     |
| 75 | 0′ °0′ °CH <sub>2</sub>                     | MAX |
|    | *Li^~jj                                     |     |
| 76 | F   | MAX |
|    | +Li- O F                                    |     |
| 77 | 0 0 0                                       | MAX |
|    | H_O_H<br>F/_1_F<br>F <b>-</b> P_ <b>-</b> F |     |
| 78 | Ė   | MAX |
|    | F   |     |
|    | 0   |     |
| 79 | †Li´  | MAX |
|    | O F   |     |
| 80 | O.\Li+                                      | MAX |
|    | F`Li+<br>P. /                               |     |
| 81 | F P F F C O O O O O O O O O O O O O O O O O | MAX |

|    | F<br><u>!</u>                           |     |
|----|---|-----|
| 82 | O P F                                   | MAX |
| 83 | F.O.                                    | MAX |
|    | .O. ^ .P.                               |     |
| 84 | +Li/ O O F                              | MAX |
| 85 | F P F                                   | MAX |
| 86 | F 0 F                                   | MAX |
| 87 | F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 | 4   |

Table 1: Principal molecules used for fragmentation, including depth of fragmentation. A fragmentation depth of "MAX" indicates that all possible combinations of bonds were broken during fragmentation.