

# The Drugstore Li-Ion Cell

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Lithium-ion batteries store the greatest energy per volume or per mass of any rechargeable battery technology compatible with portable electronics. They have excellent performance and storage characteristics, long charge-discharge cycle life, no memory effect, and are available at low cost. As such, they have become the power source of choice for portable electronic devices like laptop computers, cell phones, digital cameras, etc. On November 2, 2005, an article in the *Wall Street Journal* (New Type of Battery Offers Voltage Aplenty—at a Premium, William M. Bulkeley) described the inroads that Li-ion cells are making in markets that require high power, for example, cordless power tools. According to the article, Milwaukee Electric Power Tool has introduced a line of 28 V cordless power tools powered by lithium-ion batteries made by a Canadian unit of Taiwan's E-One Moli Energy Corp. Black and Decker and Robert Bosch GmbH are set to introduce Li-ion powered tools in early 2006. The new Li-ion cells are based on positive electrodes of either  $\text{LiMn}_2\text{O}_4$  or  $\text{LiFePO}_4$  instead of the standard  $\text{LiCoO}_2$  normally found in computer and cell-phone batteries. This is because  $\text{LiMn}_2\text{O}_4$  and  $\text{LiFePO}_4$  offer significant safety advantages over  $\text{LiCoO}_2$ <sup>1</sup> that become critical in batteries designed for high power applications.

Despite the success of Li-ion cells in computer, cell phone, and power tool applications, throwaway primary batteries like alkaline (e.g., Duracell, Energizer, etc.) still dominate applications in low cost devices like flashlights, disc players, etc. As resources become scarce, it will be responsible and cost-effective to move to rechargeable batteries for these applications. Nickel-cadmium and nickel-metal hydride batteries have been available for consumer applications for many years, but these batteries suffer from relatively rapid self-discharge and the memory effect, which reduces the capacity of cells that are continually charged. Nickel-based cells have not displaced throwaway cells in consumer applications.

Given the advantages of lithium-ion cells, one must wonder why they

have not been marketed as single cells for consumer applications. There are several reasons for this. First,  $\text{LiCoO}_2$ /graphite Li-ion cells must be charged to a specified upper cutoff potential, and not beyond, to maintain their cycle life and safety characteristics. In series-connected batteries, this cannot be ensured, unless each cell potential is monitored and controlled electronically, a practice that is used in batteries for laptop computers, for example.

Second, lithium-ion cells are not tolerant to overdischarge, a condition that occurs when a cell is discharged beyond its normal discharge end point. Consider three lithium-ion cells at arbitrary states of charge, maybe two fully charged and one 50% discharged. If these are connected in series and

then connected to a device like a flashlight, the partially discharged cell will reach end of discharge before the other two and be forced into polarity reversal by the other cells if the flashlight is left turned on. Although this does not necessarily cause a safety hazard, it forces electrodes outside their normal potential ranges and adversely affects the cycle life of the overdischarged cell and hence the battery pack. One could argue that only cells at exactly the same state of charge should ever be assembled into a series-connected battery, but this is impossible to ensure if consumers, for example, are assembling batteries in flashlights themselves.

In this article, we show recent research progress in additives to Li-ion cells that can prevent damaging overcharge and overdischarge reactions altogether. In principle, such additives may yield Li-ion cells that are virtually indestructible and cannot be damaged in low-rate applications involving consumer-assembled batteries. Such cells would be suitable for the drugstore and supermarket shelves!

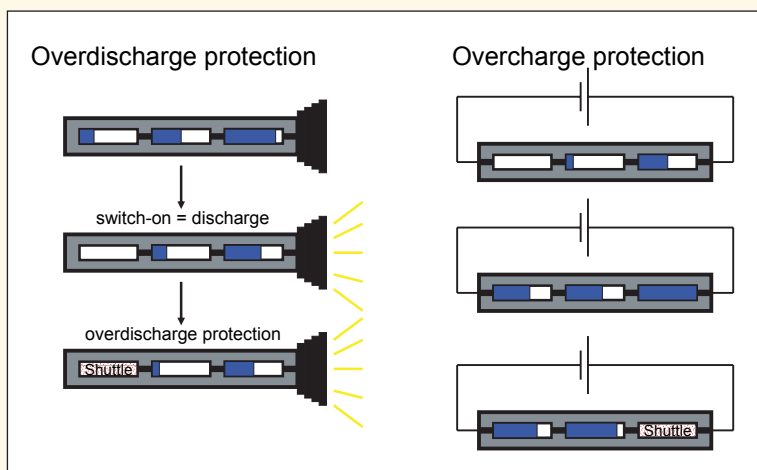
## Desired Operation of the Redox Shuttle Additive

Figure 1 shows a schematic of the desired operation of an overdischarge and overcharge protecting additive. The left panel of Fig. 1 shows three cells at arbitrary states of charge (blue corresponds to state of charge) taken from storage and placed into a series string in a flashlight (top left panel). As the flashlight operates, the cell on the left reaches the fully discharged state first (middle left panel). If the flashlight is left on, the other two cells will drive the cell on the left into potential reversal. As shown later in the article, a redox shuttle additive added to the cell prevents extremes of potential reversal and prevents damage to the leftmost cell (bottom left panel).

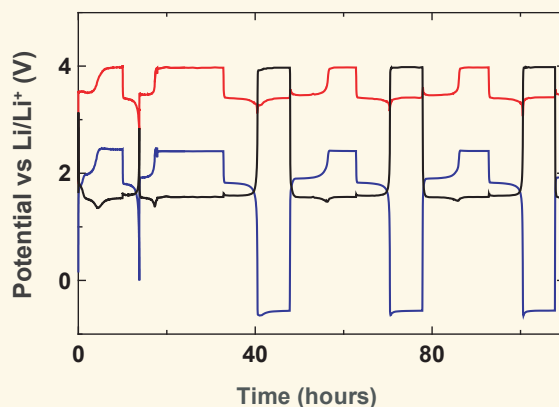
The right half of Fig. 1 shows the desired operation of the additive during a situation where three unbalanced cells are placed in a series string and then charged (top right panel). During charging, the rightmost cell reaches full state of charge first (middle right panel) and the shuttle additive functions to prevent damage while the other two cells reach full charge (bottom right panel).

The idea of a redox shuttle additive to the electrolyte of lithium batteries is not a new one,<sup>2-11</sup> but only recently have shuttle molecules with acceptable stability been found<sup>12-17</sup> that can provide overcharge and overdischarge protection for many cycles. A suitable

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**Fig. 1.** (Left) The operation of a redox shuttle to protect the cell initially at the lowest state of charge (leftmost cell) from damage during forced overdischarge. (Right) The operation of a redox shuttle to protect the cell initially at the highest state of charge (rightmost cell) from damage during forced overcharge.



**Fig. 2.** Potential vs. time for a  $\text{LiFePO}_4/\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  cell charged and discharged using constant currents ( $C/5$  for time less than 33 h and  $C/10$  for time greater than 33 h). Blue, terminal voltage of the  $\text{LiFePO}_4/\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  cell. Red,  $\text{LiFePO}_4$  potential vs. a Li metal reference electrode. Black,  $\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  potential vs. a Li metal reference electrode. Notice that each electrode is constrained within the potential window between 1.5 and 4.2 V, even though the cell is being purposely overcharged and overdischarged.

shuttle molecule, S, can be reversibly oxidized to  $S^+$  at a potential a few hundred millivolts more positive than the normal end-of-charge potential of the positive electrode. For example,  $\text{LiFePO}_4$  and  $\text{LiMn}_2\text{O}_4$  electrodes reach the fully charged state near 3.5 and 4.1 V vs.  $\text{Li/Li}^+$ , respectively, and require shuttles that have redox potentials near 3.9 and 4.5 V, respectively. During overcharge of a Li-ion cell containing a shuttle additive, the positive electrode surpasses the usual end of charge potential and reaches the redox potential of the shuttle molecule. At this point, shuttle molecules are oxidized to  $S^+$ , which diffuse to the negative electrode and are reduced back to the neutral molecule, S. Thus,

during overcharge the oxidized shuttle molecules carry the current supplied to the cell.

The maximum current,  $I_{\text{max}}$ , that the shuttle can carry depends on several simple factors. References 2 and 3 show that  $I_{\text{max}} = n A C D F/L$ , where  $n$  is the number of charges carried by the molecule (usually  $n = 1$ ),  $A$  is the electrode area,  $C$  is the concentration of the molecule in the electrolyte,  $D$  is the diffusion constant of the shuttle molecule,  $F$  is Faraday's number, and  $L$  is the interelectrode spacing. Practical values of these parameters for typical aromatic shuttle molecules, dissolved in polar nonaqueous electrolytes, may be  $C = 1 \times 10^{-4}$  mol/cm<sup>3</sup>,  $D = 1 \times 10^{-6}$  cm<sup>2</sup>/s, and  $L = 5 \times 10^{-3}$  cm. These give

a maximum shuttle current density of about 2 mA/cm<sup>2</sup>, which corresponds roughly to a C or C/2 rate for typical Li-ion cells.<sup>14</sup>

If the shuttle current density is 2 mA/cm<sup>2</sup>, each shuttle molecule makes the transit between the electrodes as an oxidized species about once every 30 s! Thus the oxidized species must be extremely stable in the electrolyte and also at each electrode in order to protect Li-ion cells under conditions of repeated overcharge and overdischarge. There are thousands of aromatic (and other) molecules that show reversible redox reactions as measured on the time scales of cyclic voltammetry.<sup>18</sup> However, as discussed below, few actually have the required stability.

### Actual Operation of a Redox Shuttle Additive

Figure 2 shows the operation of a  $\text{LiFePO}_4/\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  Li-ion cell containing 0.1 M 2,5-di-*tert*-butyl-1,4-dimethoxybenzene (DDB) (redox potential = 3.92 V vs.  $\text{Li/Li}^+$ ) during a cycling regime where the cell was deliberately forced into overcharge and overdischarge repeatedly. The blue curve shows the cell terminal voltage vs. time. The normal charge-discharge plateau is 1.9 V for this cell because the  $\text{LiFePO}_4$  positive and  $\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  negative electrodes have potentials of 3.45 and 1.55 V vs.  $\text{Li/Li}^+$ , respectively. When the cell reaches full charge, the terminal voltage increases steeply until the shuttle operates (at a terminal voltage of 2.4 V) while the current continues to flow. Similarly, when the cell reaches end of discharge, the terminal voltage decreases rapidly until the shuttle begins to operate (at a terminal voltage of about -0.5 V) while current continues to flow. The black and red curves, respectively, show the potential of each of the positive and negative electrodes measured vs. a Li metal reference.

Clearly, during overcharge, the positive electrode reaches the shuttle potential and is clamped there. During the overdischarge, the negative electrode surpasses the potential of the positive electrode as the cell goes into reversal, but then the negative electrode is clamped at the shuttle potential as well. For this cell, it is impossible to move either electrode outside its electrochemical stability window, even if 100% overcharge or overdischarge capacities are applied as in Fig. 2.

### How Many Molecules Can Support Reversible Shuttle Behavior?

A simple screening test that we have initiated in our laboratory is continual C/10 cycling of  $\text{LiFePO}_4/$

$\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  coin-type cells containing 0.1 M shuttle additive where each charge cycle is constrained to last for 20 h, even though a 10 h period would completely charge the cell. This repeated 100% overcharging quickly identifies molecules that do not have the required stability. Figure 3 shows

a histogram of the number of 100% overcharge cycles supported before shuttle capability ceases. Out of more than 60 molecules tested, only three molecules, 10-methylphenothiazine (MPT), 2,2,6,6-tetramethylpiperidine 1-oxyl (TEMPO), and DDB supported more than 100 overcharges.<sup>15,17</sup>

Therefore, long-term stability of the oxidized shuttle molecule in the reaction cocktail of the electrolyte is not the norm.

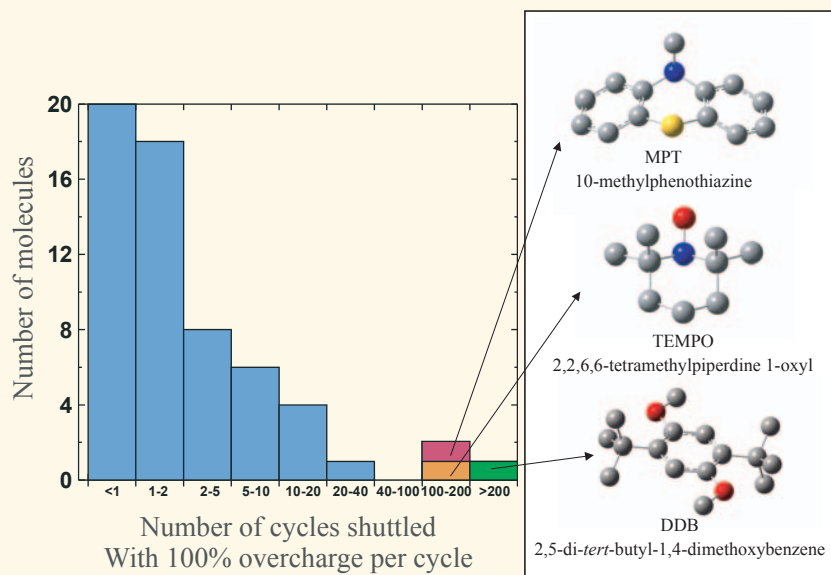
### Use of the DDB Shuttle in 18650 Size Cells

Given the success of the DDB shuttle, collaborations with a Li-ion battery manufacturer were initiated so that 18650 size  $\text{LiFePO}_4/\text{graphite}$  Li-ion cells containing DDB shuttle could be tested. Sixty cells were manufactured and studied with a battery of tests.<sup>19</sup> As an example of the successful operation of the shuttle, Fig. 4 shows extended charge-discharge cycling of three-cell series-connected batteries of  $\text{LiFePO}_4/\text{graphite}$  18650 size cells. The battery described by the graphs on the left had a 330  $\Omega$  resistor placed across one cell. During each charge, the other two cells in this pack operated in shuttle-protected overcharge for about 1 h before the self-discharging cell became fully charged (lower left graph of Fig. 4). This successful operation occurred for the full 2800 h of this test. The battery described by the graphs on the right did not incorporate any resistors. Figure 4 also shows that the shuttle in the battery with the resistor across one cell and the shuttle in the battery incorporating no resistor show equivalent cycle life. Figure 4 clearly shows that the DDB shuttle can protect  $\text{LiFePO}_4/\text{graphite}$  cells from being driven into overcharge in deliberately unbalanced batteries.

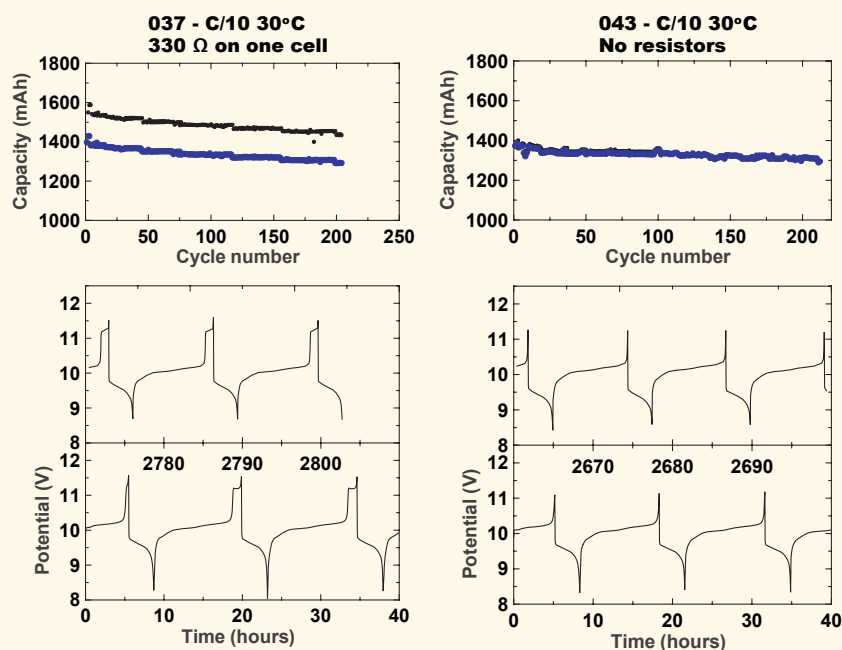
### Theoretical Methods to Guide the Search for New Shuttle Molecules

In a recent paper, Wang *et al.*<sup>16</sup> systematically performed quantum chemical calculations (using Gaussian ver. 03™<sup>20</sup>) on candidate shuttle molecules to evaluate their oxidation potentials. Figure 5 compares the theoretical and experimental results for the oxidation potentials for 17 molecules, covering four classes of molecules: eight aromatic molecules, three TEMPO or 2,2,6,6-tetramethylpiperidinyloxy-like radicals, three pyridine N-oxide-like molecules, and three N-substituted phenothiazine molecules. The agreement between the calculation and experiment is good. With such precision, quantum chemical calculations become a powerful tool in the processes of searching for new redox shuttle candidates. Molecules with calculated oxidation potentials out of the desired range can be eliminated before experiments are even performed. Existing molecules can be modified by

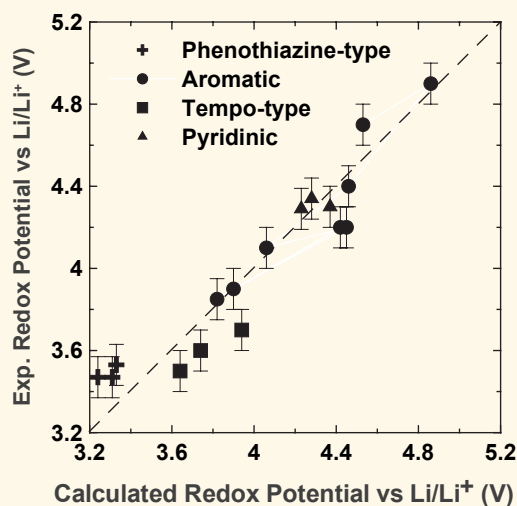
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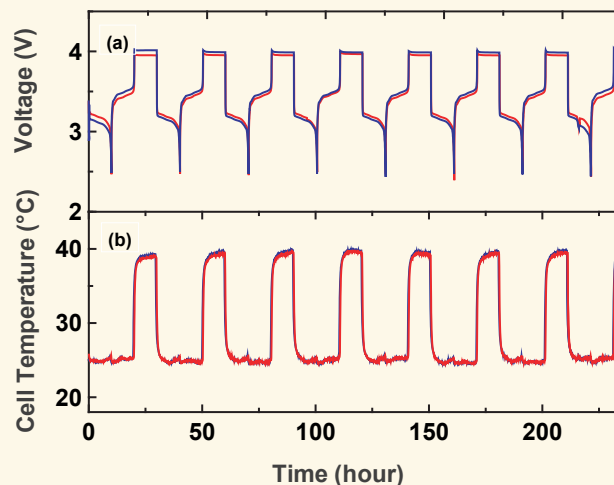
**FIG. 3.** The histogram shows the number of 100% overcharge cycles in  $\text{LiFePO}_4/\text{Li}_{4/3}\text{Ti}_{5/3}\text{O}_4$  cells that 60 different redox active molecules can support. Only three molecules (at right) could support more than 100 overcharge cycles. (Hydrogen atoms are not shown.)



**FIG. 4.** Extended charge-discharge cycling of three-cell series-connected batteries of  $\text{LiFePO}_4/\text{graphite}$  18650 size cells. The battery described by the graphs on the left had a 330  $\Omega$  resistor placed across one cell. During each charge, the other two cells in this pack operated in shuttle-protected overcharge for about 1 h before the self-discharging cell became fully charged (lower left graph) for the full 2800 h of this test. The battery described by the graphs on the right did not incorporate resistors. The battery with the resistor across one cell and the battery incorporating no resistor show equivalent cycle life (top panels) [black, charge capacity; blue, discharge capacity].



**Fig. 5.** Experimental shuttle redox potential plotted vs. redox potentials calculated using Gaussian 03 and the method described in Ref. 16.



**Fig. 6.** (a) Cell terminal voltage and (b) cell surface temperature vs. time for two 18650 size LiFePO<sub>4</sub>/graphite cells charged and discharged using a current of 140 mA (C/10). During shuttle-protected overcharge, the  $I V$  power supplied to the cell appears entirely as heat and the cell temperature rises by about 14°C.

ligand substitution to tune the redox potential, for example, see Ref.15. Using the methods described in Ref. 16 the redox potentials may be estimated theoretically before their synthesis is undertaken. There is no doubt that this saves resources and speeds the research process in this laboratory.

It is our hope that theoretical methods may be used to estimate the stability of the oxidized shuttle molecule in the reaction cocktail of the electrolyte. This is extremely important because there are many molecules that show approximately the desired oxidation potentials (3.9 V for LiFePO<sub>4</sub> positive electrodes and 4.5 V for LiMn<sub>2</sub>O<sub>4</sub> positive electrodes) but very few (see Fig. 3) that show the required stability.

#### Other Approaches to Overcharge Protection

In recent work,<sup>21</sup> Dantsin *et al.* described weakly coordinating perfluoroborane cluster salts, *i.e.*, lithium fluorododecaborates (Li<sub>2</sub>B<sub>12</sub>F<sub>x</sub>H<sub>12-x</sub>) that not only function as the electrolyte salt but also as a redox shuttle. The doubly charged anion, B<sub>12</sub>F<sub>x</sub>H<sub>12-x</sub><sup>2-</sup> can be oxidized to the singly charged anion at about 4.5 V. Therefore the salt's unique oxidation chemistry also provides inherent protection against overcharge and may be well-suited to the LiMn<sub>2</sub>O<sub>4</sub> positive electrode. Equally interesting is that the redox potential is tunable by controlling the degree of fluorination (*i.e.*,  $x$  in B<sub>12</sub>F<sub>x</sub>H<sub>12-x</sub>)

in the fluorododecaborate anion. Molecules with a smaller value of  $x$  (less fluorine) have a lower redox potential. Dantsin *et al.*<sup>21</sup> showed that small test cells incorporating this salt exhibited shuttle-protected overcharge for an equivalent of 100 times the nominal cell capacity at C rate. Salts of this type that provide more than a single function, are very interesting to lithium battery researchers.

In other recent work, Chen *et al.*<sup>22,23</sup> described the use of a redox active polymer incorporated into the separator of a Li-ion cell to provide overcharge protection. Basically, once the redox potential of the polymer is exceeded, the electrical conductivity of the polymer increases by many orders of magnitude and overcharge is prevented. Chen *et al.*<sup>23</sup> demonstrated that reliable and reversible overcharge protection could be achieved in a test-scale lithium battery by incorporating an electroactive polymer, poly(3-butylthiophene) or P3BT, within the porous separator membrane without filling a large number of the pores. Oxidation of this polymer during overcharge generates an internal short which allows an overcharge current to pass harmlessly through the cell, while the subsequent reduction of the polymer on cessation of overcharging restores the polymer to its insulating state, and allows the cell to be discharged normally. This approach requires the engagement of separator manufacturers, who must incorporate the desired polymers

within their products, before widespread use may be achieved.

#### Heat Generation during Shuttle-Protected Overcharge and Overdischarge

During the operation of the shuttle process in either overcharge or overdischarge, there is no work being done on the electrodes. Therefore the electrical power supplied to the cell by the charger,  $I_{app} V_{cell}$ , appears directly as heat. Figure 6 shows the cell terminal voltage and cell surface temperature vs. time for two 18650 size LiFePO<sub>4</sub>/graphite cells charged and discharged using a current of 140 mA (C/10). During shuttle-protected overcharge, the  $I_{app} V_{cell}$  power supplied to the cell appears entirely as heat and the cell temperature rises by about 14°C. If the charging current doubles, the thermal power doubles and the temperature rise above ambient also doubles (according to Newton's law of cooling). Therefore, for a LiFePO<sub>4</sub>/graphite 18650 cell charged at C rate, the cell surface temperature increases by about 140°C as the shuttle operates, provided that only ambient cooling is used.

All overcharge protection strategies described in the previous sections will generate  $I_{app} V_{cell}$  heat during shuttle protected overcharge and overdischarge. This immediately suggests that the use of an internal redox shuttle is not a good strategy for balancing long series strings of cells that may be found in hybrid

vehicle battery packs where charging rates of up to 40C during regenerative braking are imagined. Instead, modest charging rates, like overnight charge, are well-suited to the internal redox shuttle approach. With reference to Fig. 1, 2, and 6, extended shuttle-protected overcharging at C/10 rate would not create thermal problems for 18650 size cells. Furthermore, if such cells exhibit shuttle-protected overdischarge, the heat generation is about eight times less, because the cell terminal voltage has a magnitude of only about 0.5 V, and thus could support C-rate shuttle-protected overdischarge without significant heating. This suggests that a shuttle protected Li-ion cell is well-suited to consumer applications, like flashlights, disc players, cameras, etc.

For redox shuttle overdischarge protection in Li-ion cells to be a reality, the current collector normally used for the negative electrode, copper, must be changed. This is because copper dissolves at the oxidation potential of shuttles required to protect LiFePO<sub>4</sub> and LiMn<sub>2</sub>O<sub>4</sub> positive electrodes. This suggests that research on inexpensive corrosion-resistant current collectors that can tolerate both lithium potential and potentials near 4.5 V is a priority.

### Concluding Remarks

It is our opinion that long-lasting redox shuttles can be found that are suitable for almost any Li-ion chemistry. These shuttles can be used (as in Fig. 2) to keep both electrodes in potential ranges where they are completely stable. Hence, such a shuttle-protected Li-ion cell, incorporating a LiFePO<sub>4</sub> or LiMn<sub>2</sub>O<sub>4</sub> positive electrode, should be virtually immune to damage due to unintentional overcharge or overdischarge and would therefore probably be suitable for sale over-the-counter in drugstores, supermarkets, and the like. [As was noted, however, the benefits of the shuttle are restricted to relatively low rates to avoid overheating while the shuttle operates.] The addition of such stable shuttles does not adversely affect the cycle life and performance of the cell to which it is added (Fig. 4). Therefore Li-ion cells containing a redox shuttle additive should be virtually electrically indestructible.

Imagine a battery that outlives the flashlight in which it is placed, and can be used in flashlights for several generations. Imagine leaving cells and batteries to your offspring in your will because they last forever and cannot be damaged unintentionally. It is our

opinion that this situation is not far away. Furthermore, in a world with finite resources, batteries with longer lifespan are a necessary alternative to throwaway batteries.

### Acknowledgments

The authors acknowledge NSERC, 3M Co., and the Canadian Institute of Advanced Research for the funds to carry out the work described above. The authors gratefully acknowledge Dr. Qiming Zhong of E-One Moli Energy Canada Ltd. for the 18650 size LiFePO<sub>4</sub>/graphite cells containing DDB. Dr. Kevin Eberman, Dr. Larry Krause, and Dr. Mark Obrovac of 3M Co. are acknowledged for their support of this work. ■

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