The Li-Air Battery – Opening Up for Electric Vehicle Applications

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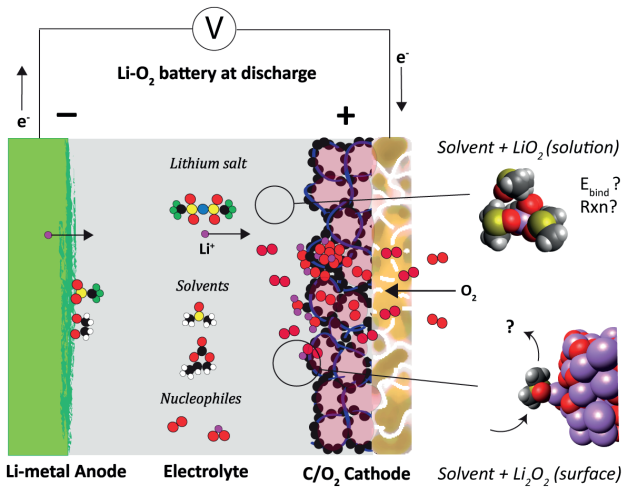
The so-called Li-ion battery is an energy storage technology that has paved the way for smart-phones and a plethora of other portable electronics. The highly energetic, reversible, and fast transport of ions (Li^+) between two inert host electrodes, via a non-aqueous medium, makes these batteries ideal for the purpose. However, targeting new applications such as to store and deliver energy for electric vehicle propulsion identifies hurdles that will not be easily met by any Li-ion battery.

For electric vehicles to be truly competitive with conventional vehicles, the batteries for the former must provide a cost, safety, and driving range that are comparable to that provided for the latter by gasoline. At an energy density of ~200 Wh/kg, Li-ion batteries are far off from the ~1700 Wh/kg extractable from gasoline. Therefore, substantial improvements in energy density, as well as cost, must be explored in "new" battery technologies.

Guided by the principle "*more from less*", the Li-air battery uses oxygen from the surrounding as fuel for one of the electrode reactions. Contrary to the Li-ion battery, the Li^+ is not transported passively between the electrodes, but reacts with O_2 at the cathode to form Li_2O_2 or LiO_2. The conversion reaction, together with a low cathode mass and a Li-metal anode, offers the ability for abrupt changes in properties vs. the Li-ion battery – in particular an estimated practical energy density of the order 1000 Wh/kg. Key to success will be to master the reversibility of the chemical reactions involving Li^+.

The major technological hurdles to develop Li-air batteries include identifying materials that do not react with the intermediate (dissolved) or final (solid) reduction products of O_2, since the reversibility of the reactions are strongly dependent on minimizing side-reactions. Another challenge is to selectively pass O_2 from air into the cathode, because low levels of moisture or carbon dioxide will quickly deteriorate battery performance. This must be done with minimal need for additional equipment.



Schematic illustration of a Li-air battery and its components at discharge (left) and examples of sub-systems that can be explored by computational modelling (right).

With computational modelling it is possible to address the molecular level challenges, initially of Li-O_2 batteries, by selectively choosing and investigating idealized systems at different levels of detail/magnification. For this purpose we combine classic and *ab initio* molecular dynamics with static calculations of material properties.

Energy barriers to the reaction of reduced oxygen species with solvents and salts of the ion-conducting electrolyte can be predicted, and *reaction products* proposed, to later aid their experimental identification in bulk electrolyte or at electrode surfaces. "*Additives*" for modifying the interactions/reactions of the electrolyte, alternative *reaction mechanisms* at surfaces, and relative "*diffusion rates*" of electrolyte and oxygen in and out of nano-porous electrode particles, are examples of additional properties that can be addressed.