Inside-out investigation of Li-Ion batteries and Beyond: Theoretical and Computational Chemistry Approach

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Abstract- In recent years, rechargeable Li-ion batteries (LIBs) emerge as an important power source, and their performance highlights the adoption into the automobile electrical vehicles (EV) sector as viable alternatives to combustion engines. However, in existing batteries, material degradation at an electrode level (battery ageing & life-time) are major challenges to address for efficiency as well as safety. The exploration of new Li-ion battery materials and understanding degradation is an important focus of materials scientists, computational physicists and chemists throughout the world. LIBs for high energy or high power demands like vehicle application require high capacity, high capacity retention, high voltage operation, low cost, low weight and volume, etc. All of these requirements are deeply related to solid electrolyte interphase (SEI) layers. The main objectives of this work is to compare the existing mathematical model for degradation mechanism present in the literature and develop our understanding of reaction kinetics involved. Also discover a future alternative for (Li-S, Si, Na^+) batteries based on molecular-chemistry details of electrolyte materials involved Fig. 1 [1]. For finding such new electrode/electrolyte materials, a fuller understanding of how the materials composition (Electrolyte) interact at the molecular level, which is not investigated in great detail so far is highly recommended by considering cost-effective computational chemistry tools (DFT, MD).

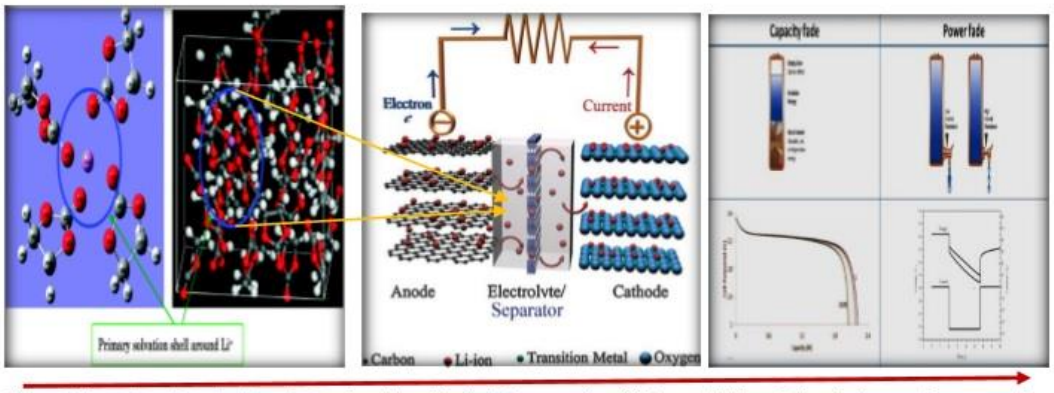

Figure 1 Overview of molecular electro-chemistry details to improve the efficiency of Li-ion Battery in terms of power and capacity fade

[1] M. Datt Bhatt and C. O'Dwyer, "Recent progress in theoretical and computational investigations of Li-ion battery materials and electrolytes," *Phys. Chem. Chem. Phys.*, vol. 17, no. 7, pp. 4799–4844, 2015.