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Structural Investigation and Cathode properties of Iron Based Oxide Glasses for Sustainable and High-Energy Density Lithium-ion Batteries

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As energy concerns grow and the society needs more sustainable and renewable energy sources, the ability to effectively store and retrieve energy is paramount. Currently, rechargeable lithium-ion batteries (LIB) seem to be one of the best alternatives to reduce our dependency on fossil fuels. LIB are made of cathodes materials based on polycrystalline oxides or polyanion compounds¹. However, some of them have their performance limited by their crystalline structure where other compounds suffer from irreversible phase changes during cycling². To overcome these key shortcomings, implement glasses as cathode materials seems to be an interesting approach. Indeed, depending on the glass composition large specific capacities can be reached³. Moreover, glasses have a structure composed of free volume that can easily accommodate structural changes upon lithium ions extraction and insertion⁴. Finally, glass production is scalable and commercially easier to implement than most of synthesis processes of conventional cathodes materials.

In this study, several iron based oxide glasses have been investigated as promising cathode materials for sustainable and high energy density LIB. The influence of the nature of the polyanion (PO_4 , SiO_4) and the synthesis conditions on the structural, electrical and electrochemical properties of the glasses were examined. Electronic and ionic conductivities were measured by Electrochemical Impedance Spectroscopy (EIS) on the bulk glasses. The electrochemical properties in terms of specific capacity, redox potentials vs Li^+/Li , first cycle capacity loss, coulombic and energy efficiencies of these materials were investigated in coin-cell (vs lithium metal) by Galvanostatic Cycling (GC). Finally, to elucidate the reaction mechanisms of the electrochemical processes involved in these materials, X-ray diffraction (XRD) and ^{57}Fe Mössbauer spectroscopy at room temperature were coupled and performed on the as-prepared glasses and on ex-situ (after cycling) materials at different electrochemical states of charge. This new study will bring significant elements to optimize both the glass composition and its elaboration conditions to obtain high performance cathode materials without critical materials.

¹Nitta, N. *et al.*, Li-ion battery materials: present and future. *Materials Today* **18**, 252–264 (2015).

²Tesfamhret, Y. *et al.*, On the Manganese Dissolution Process from LiMn_2O_4 Cathode Materials. *ChemElectroChem* **8**, 1516–1523 (2021).

³Afyon, S. *et al.*, New High Capacity Cathode Materials for Rechargeable Li-ion Batteries. *Scientific Reports* **4**, 7113 (2015).

⁴Kindle, M. *et al.*, Alternatives to Cobalt. *ACS Sustainable Chemistry Engineering* **9**, 629–638 (2021).