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SYNTHESIS OF FLUORINATED MATERIALS FOR ENERGY STORAGE : FROM HIGH-PRESSURE TO SOLID-GAS FLUORINATION

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In the last decades, fluorinated materials have attracted attention as cathode materials for secondary batteries; the high electronegativity of fluoride affords higher potentials in comparison with oxides when used as positive electrodes, but also enhanced electrochemical and mechanical properties for solid electrolytes.[1] Both applications can offer strategies to improve the performances of Lithium Ions Batteries (LIBs). High-pressure synthesis is a powerful method to discover and stabilize new fluorides with unique structures. One such strategy involves tuning the chemical composition of fluoride compounds, which offer a broad landscape for pressure-induced phase transitions. In particular, the high-pressure behavior of $Li_2M^{4+}F_6$ compounds has been shown to be correlated strongly with the ionic radius of the M^{4+} cation in six-fold coordination Li_2TiF_6 and Li_2MoF_6 were stabilized in the Li_2ZrF_6-type structure under 7.7 GPa and 3 GPa, respectively.[2] An extension to this work on trirutile with the high-pressure form of $LiFe_2F_6$ obtained by heating at 773 K under 2.7 GPa. Its structure from Rietveld refinement of the X-ray diffraction pattern (XRD) consisting of layers of [FeF_6] octahedra sharing corners and forming hexagonal tunnels for Li^+ ions.
Also, the development of non-flammable solid electrolytes appears to be the solution to improve the performances of LIBs. The solid electrolyte could form a barrier that inhibits the growth of lithium dendrites, thereby preventing contact between the two electrodes.[3] Solid electrolytes are becoming increasingly popular in research due to their recent relevance in the energy field. Fluorination of solid electrolytes is one of the strategies developed to improve their properties, particularly their electrochemical performance. Fluorination using Xenon difluoride (XeF_2) has emerged as a promising technique for optimizing the properties of solid electrolytes, especially in terms of ionic conductivity and electrochemical stability.[4]

References

1: Hyrondelle, H., Terry, A., Lhoste, J., Tencé, S., Lemoine, K., Olchowka, J., Dambournet, D., Tassel, C., Gamon, J., Demourgues, A. Chem. Rev. 2025
2: Inaguma, Y., Oyanagi, M., Ueda, K. Inor. Chem. 2022
3: Yu, T.; Liang, J.; Luo, L.; Wang, L.; Zhao, F.; Xu, G.; Bai, X.; Yang, R.; Zhao, S.; Wang, J.; Yu, J.; Sun, X. Adv. Energy Mater. 2021
4: Zhou, L.; Minafra, N.; Zeier, W. G.; Nazar, L. F. Acc. Chem. Res. 2021