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Surface reactivity of layered manganese oxides: an experimental and theoretical approach

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Electrochemical storage of energy through Li ion devices is the commonly used solution to address the intermittent character of renewable energy and the increasing demand of nomad technologies. LiCoO_2 is the most widely used positive electrode material of today's Li ion batteries. In the last decade, much research has been performed to explore alternative materials as mixed transition metal oxides $\text{LiNi}_x\text{Mn}_x\text{Co}_{1-2x}\text{O}_2$ (NMC). The surface reactivity of these electrode materials towards the electrolyte is a key feature that has deep impact on the performance and lifetime of Li-ion cells and need to be understood and controlled. Within this framework, based on our previous experience on lithium layered oxides, we decided to study the surface reactivity of Li_2MnO_3 which can be viewed as a model compound for Mn(IV) layered oxides such as NMC or even Li rich materials. The strategy consists coupling adsorption of gaseous probe molecule (SO_2), X-ray photoelectron spectroscopy

(XPS) and DFT calculation in order to identify the influence of the oxidation state of the transition metal on the adsorption reaction type (basic/acidic or redox). We focus our study on strengthening the experimental calculation coupling by studying the reactivity on a single crystal surface of Li_2MnO_3 . Both approaches conclude to a redox adsorption mode with the formation of sulphate species. Chemical maps of the crystal surface after adsorption obtained by Auger spectroscopy provide information on the adsorption sites location. Stacking faults and spinel type defect are usually encountered in the Li_2MnO_3 crystals. Thus, we completed this study with the investigation of the surface reactivity of Li_2MnO_3 polycrystals against the stacking faults rate. Moreover, the reactivity of $\text{Li}_{1+x}\text{Mn}_{2-x}\text{O}_4$ spinel materials will be checked to determine the influence of the spinel type defect on the surface reactivity.

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