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

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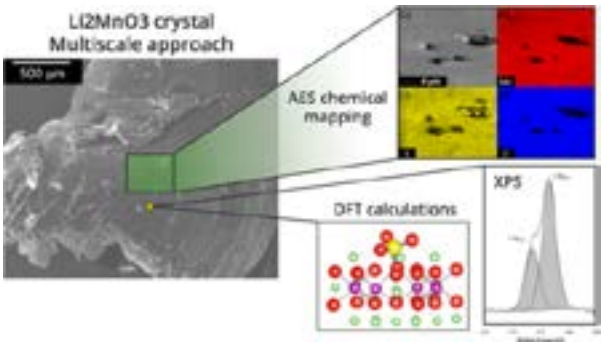
Electrochemical storage of energy through Li-ion devices is the commonly used solution to address the intermittent character of renewable energy and the increasing demand of nomad technologies. $LiCoO_2$ is the most widely used positive electrode material of today's Li-ion batteries. In the last decade, much research has been performed to explore alternative materials as mixed transition metal oxides $LiNi_xMn_xCo_{1-2x}O_2$ (NMC). The surface reactivity of these electrode materials towards the electrolyte is a key feature that has a deep impact on the performance and lifetime of Li-ion cells and needs to be understood and controls. 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 view as a model compound for Mn^{IV} layered oxides such as NMC or even Li-rich materials. The strategy consists in 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 default 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 $Li_{1+x}Mn_{2-x}O_4$ spinel materials will be checked to determine the influence of the spinel type default on the surface reactivity.



Recent Publications:

1. Quesne-Turin, A. et al. Morphology and Surface Reactivity Relationship in the $Li_{1+x}Mn_{2-x}O_4$ Spinel with x = 0.05 and 0.10: A Combined First-Principle and Experimental Study. ACS Appl. Mater. Interfaces 2017, 9 (51), 44922–44930.
2. Quesne-Turin, A. et al. Surface Reactivity of Li_2MnO_3: First-Principles and Experimental Study. ACS Appl. Mater. Interfaces 2017, 9 (50), 44222–44230.
3. Vallverdu, G. et al. First Principle Study of the Surface Reactivity of Layered Lithium Oxides $LiMO_2$ (M = Ni, Mn, Co). Surface Science 2016, 649, 46–55.
4. Guille, É. et al. Possible Existence of a Monovalent Coordination for Nitrogen Atoms in LixPOyNz Solid Electrolyte: Modeling of X-Ray Photoelectron Spectroscopy and Raman Spectra. J. Phys. Chem. C 2015, 119 (41), 23379–23387.
5. Martin, L. et al. First Principles Calculations of Solid–solid Interfaces: An Application to Conversion Materials for Lithium-Ion Batteries. J. Mater. Chem. 2012, 22 (41), 22063–22071.

Biography

Germain Vallverdu is associated professor in the university of Pau & Pays Adour, France at the IPREM institute (Institute of analytical sciences and physico-chemistry for environment and materials), CNRS / UPPA UMR 5254. He is a specialist in theoretical chemistry and numerical simulations. His research activities concern the development of new methods and computational strategies at different time or space scales (from quantum to classical approaches), applied to the investigations of complex systems. The computational approaches are lead in close interaction with experimentalists and take advantage of the high level instrumental platform of the institute. Examples of these systems and applications are the investigation of the chemical reactivity and the electronic properties at the surfaces and interfaces of materials used in lithium-ion cells.

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