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The role of atomic bond strengths and structural disorder in MXene materials for rechargeable ion-batteries

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Ion batteries are a key technology and play a dominant role in today's world. Extensive research efforts have been dedicated to exploring and developing new cathode materials with higher capacities and lifetimes. Recently, a new family of transition metal carbides and carbonitrides called "MXene" has been synthesized with a layered hexagonal structure and $M_{n+1}AX_n$ chemistry, where M is an early transition metal, A is an A-group element (mostly groups 13 and 14), X is carbon or nitrogen, and n=1, 2, or 3. MXenes have been found to be promising electrode materials, with capacities close to that of commercially available batteries and an excellent capability to handle high cycling rates. However, studies of correlation of their structural stability and functional properties could help to expand further theirs performances. To address this issue we have performed temperature dependent extended X-ray absorption fine structure (EXAFS) measurements at the Ti K-edge on representative members of the MXene family. Temperature dependent measurements permit to have direct access to the local force constant between the atomic pairs and correlate this information with the battery capacity and ions diffusion rate. Presented results address fundamental structural aspects that define the functional properties of electrode materials for ion batteries.

Recent Publications

1. Olszewski W, Isturiz I, Marini C, Avila M, Okubo M, Li H, Zhou H, Mizokawa T, Saini N L and Simonelli L (2018) Effects of nanostructuring on the bond strength and disorder in V_2O_5 cathode material for rechargeable ion-batteries, physical chemistry. Chemical Physics 20:15288-15292.
2. Simonelli L, Paris E, Wakita T, Marini C, Terashima K, Miao X, Olszewski W, Ramanan N, Heinis D, Kubozono Y, Yokoya T, Saini N L (2017) Effect of molecular intercalation on the local structure of superconducting Nax(NH_3)y$MoSe_2$ system, Journal of Physics and Chemistry of Solids 111: 70-74.
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4. Olszewski W, Avila Perez M, Marini C, Paris E, Wang X, Iwao T, Masashi Y, Atsuo M, Takashi S, Saini N, Simonelli L (2016) Temperature Dependent Local Structure of NaxCoO_2 Cathode Material for Rechargeable Sodium-ion Batteries, Journal of Physical Chemistry C 120: 4227-4232.
5. Paris E, Simonelli L, Wakita T, Marini C, Lee J-H, Olszewski W, Terashima K, Kakuto T, Nishimoto N, Kimura T, Kudo K, Kambe T, Nohara M, Yokoya T, Saini N (2016) Temperature dependent local atomic displacements in ammonia intercalated iron selenide superconductor, Scientific Reports 6: 27646.

Biography

Wojciech Olszewski is a Post-Doctoral Research Associate at the ALBA Synchrotron Light Facility. He studies energy materials, and the current research direction is the investigation of the structural stability, local atomic displacements and the force constants during the diffusion process for finding a realistic correlation between the local structure and functional properties of cathode materials.

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