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The role of atomic bond strengths and structural disorder in cathode 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. The presented results address fundamental structural aspects that define the functional properties of cathode materials for ion batteries.

Recent Publications

1. Simonelli L, Paris E, Wakita T, Marini C, Terashima K, Miao X, Olszewski W, Ramanan N, Heinis D, Kubozono Y, Yokoya T and Saini N L (2017) Effect of molecular intercalation on the local structure of superconducting Nax(NH3)yMoSe2 system. Journal of Physics and Chemistry of Solids 111:70-74.
2. Szymanski K, Olszewski W, Satuła D, Gawryluk D J, Krzton-Maziopa A and Kalska-Szostko B (2017) Determination of hyperfine fields orientation in nuclear probe techniques. Spectrochimica Acta A 173:827–831.
3. Broux T, Bamine T, Fauth F, Simonelli L, Olszewski W, Marini C, Ménétrier M, Carlier D, Masquelier C and Croguennec L (2016) Strong impact of the oxygen content in Na3V2(PO4)2F3-yOy (0≤y≤0.5) on its structural and electrochemical properties. Chemistry of Materials 28:7683–7692.
4. Olszewski W, Avila Perez M, Marini C, Paris E, Wang X, Iwao T, Masashi Y, Atsuo M, Takashi S, Saini N and Simonelli L (2016) Temperature dependent local structure of NaxCoO2 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 and Saini N (2016) Temperature dependent local atomic displacements in ammonia intercalated iron selenide superconductor. Scientific Reports 6:27646.

Biography

Wojciech Olszewski is a Postdoctoral Research Associate at the ALBA Synchrotron Light Facility. He studies energy materials, and his 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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