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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 [1]. Extensive research efforts have been dedicated to exploring and developing new cathode materials with higher capacities and lifetimes [2].
Recently, a new family of transition metal carbides and carbonitrides called "MXene"has been synthesized with a layered hexagonal structure and M_{n+1}X_n chemistry, where M is an early transition metal, X is carbon or nitrogen, and n=1, 2, or 3 [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 [4]. 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 [5,6]. Presented results address fundamental structural aspects that define the functional properties of electrode materials for ion batteries.

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