

CYCLE DE CONFÉRENCES DE CHIMIE

Avec le concours de : Université Clermont Auvergne
SIGMA Clermont

Lundi 2 décembre à 16 h

Amphi Rémi (site des Cézeaux)

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Model materials for multivalent ion batteries

From the perspective of the ionic radius, multivalent ions (MV) such as Mg^{2+} , Ca^{2+} and Al^{3+} exhibit ionic radii than are close to Li^+ or Na^+ , and thus the insertion of such cations in host frameworks is, in principle, achievable. Other characteristics of the charge carriers, however, must also be taken into account, in particular, the extent to which the cation interacts with the anionic sublattice. The polarizing power (Z/r^2 where Z is the charge of the ion and r is its radius in Å) reflects the ability of a cation to attract and distort the electron cloud of a nearby anion. By comparing values of the polarizing power between Li^+ and Al^{3+} cations, we can expect an increasing interaction with the anionic sublattice moving from Li^+ ($1.73 \text{ e } \text{\AA}^{-2}$) to Al^{3+} ($10.68 \text{ e } \text{\AA}^{-2}$). As a consequence, the intercalation chemistry of MV ions is expected to strongly differ from that typically encountered for the lithium-ion.¹ So far, knowledge's on MV intercalation chemistry remains poorly understood because of several limitations including a limited number of suitable frameworks that enabled MV intercalation. Here, we will present and discuss two Ti-based compounds recently reported by us²⁻⁴ that are prone to accommodate MV ions. These compounds that are based on 3D-anatase and layered-like lepidocrocite (Figure 1) type structures have specific structural features that enabled to reversibly insert MV ions. The specific features of MV intercalation chemistry will be critically discussed.⁵

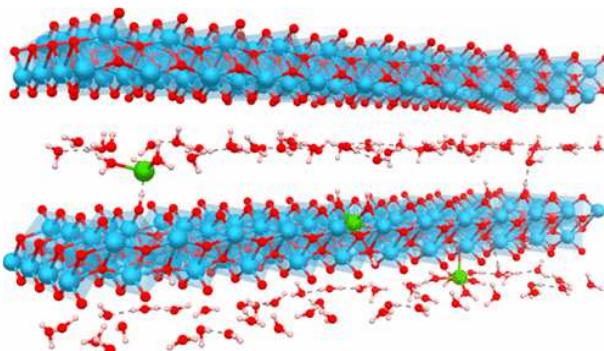


Fig. 1 Representation of the Lepidocrocite structure.

References

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- (2) Li, W.; Corradini, D.; Body, M.; Legein, C.; Salanne, M.; Ma, J.; Chapman, K. W.; Chupas, P. J.; Rollet, A.-L.; Julien, C.; et al. High Substitution Rate in TiO_2 Anatase Nanoparticles with Cationic Vacancies for Fast Lithium Storage. *Chem. Mater.* 2015, 27 (14), 5014–5019. <https://doi.org/10.1021/acs.chemmater.5b01407>.

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