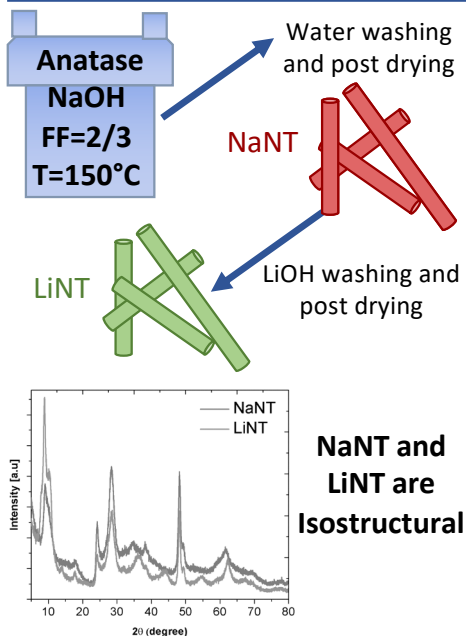


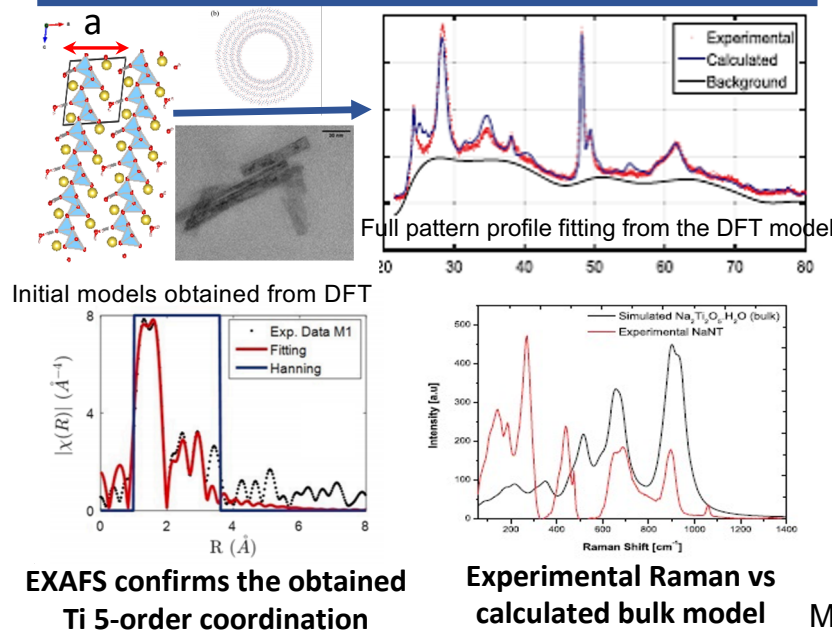
Na- and Li-ion titanates for energy applications

M. Esteves, L. Amy, L. Fernández-Werner, A. W. Mombrú, S. Favre & R. Faccio*

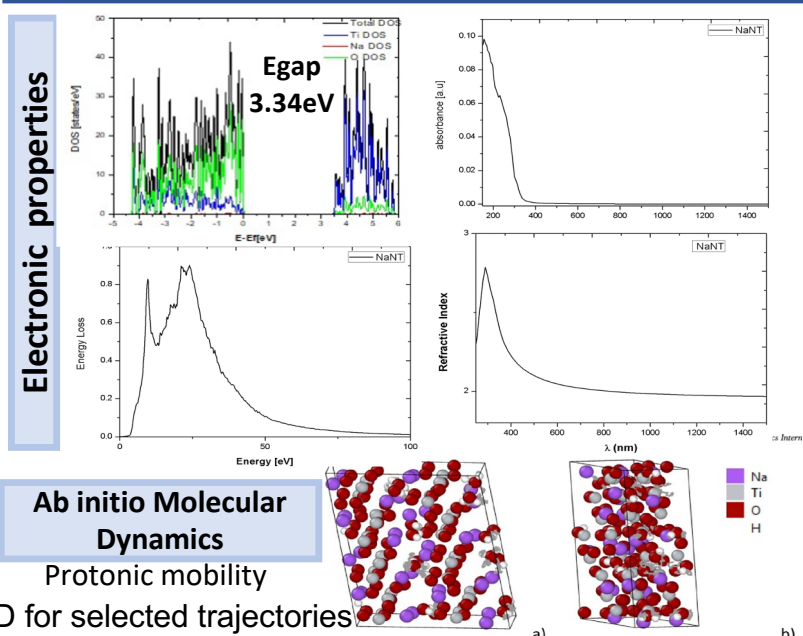
Synthesis



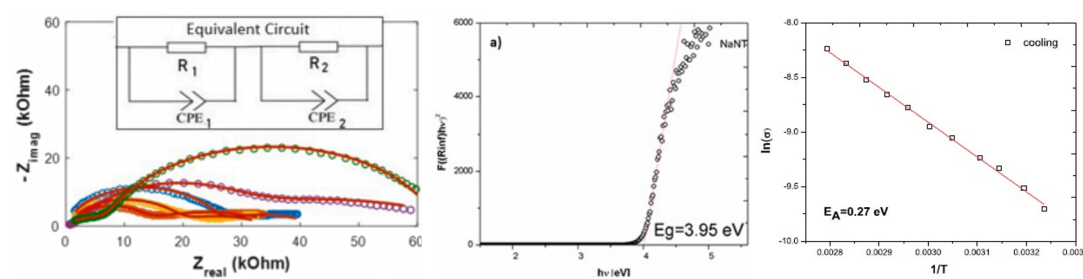
Structural characterization



DFT+U Modeling (GGA+U)



Electronic characterization



Conclusions

This work presents the complete structural characterization of $\text{Na}_2\text{Ti}_2\text{O}_5$ nanotubes and by analogy $\text{Li}_2\text{Ti}_2\text{O}_5$ nanotubes. The DFT models are capable of explaining and predicting the exhibited optical and electronic properties. Electric properties were studied in terms of EIS, distinguishing two main ionic process, in which one of them is not reversible with temperature. It is worth noticing that also protonic conduction should be considered when studying the ionic transport in the samples.

[1] M. Esteves, et.al. Optical, electrical and structural properties of Fe doped sodium titanate nanostructures, Appl. Surf. Sci., 552 (2020) 149534.

[2] L. Amy, et.al. The effect of morphology on the optical and electrical properties of sodium titanate nanostructures., Appl. Surf. Sci., (2021).

[3] M. Esteves, et.al. A step forward towards the structural characterization of $\text{Na}_2\text{Ti}_2\text{O}_5 \cdot \text{H}_2\text{O}$ nanotubes and their correlation with optical and electric transport properties, Ceram. Int., 46 (2020) 2877- 2886.

[4] F. Pignatelli, et.al. Lithium titanate nanotubes as active fillers for lithium-ion polycrylonitrile solid polymer electrolytes, Ionics, 25 (2018) 2607-2614.