Combining X-ray spectroscopies and first principles theory for the study of metal insulator transitions in transition metal oxides

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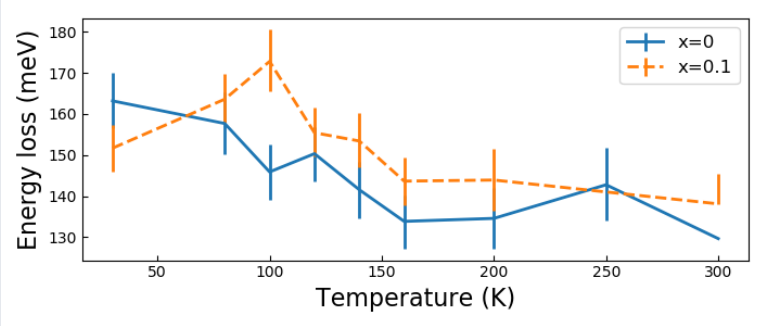
The main purposes of our project was to perform a study of the metal insulator transition in $La_{1-x}Sr_xVO_3$ [1] thorough resonant inelastic X-ray scattering (RIXS) [2] and non-resonant inelastic X-ray scattering (IXS), in order to both provide insight into the phase diagram of $La_{1-x}Sr_xVO_3$ and to provide a solid data set for theory development. Transition metal oxides exhibit partially filled narrow bands and electron correlation effects are significant. Thus advanced methods of many-body theory are required to understand their properties. As the target of study and the method are both complicated, it is desirable to interpret experiments carefully using first principles theory. **The resonant scattering cross section is naturally more complicated for theory than the non-resonant case**, hence combining RIXS and non-resonant IXS is particularly interesting as the IXS cross section is theoretically well understood [3].

We performed several experiments at Synchrotron Soleil and the European Synchrotron Radiation Facility characterizing the metal to insulator transition in $La_{1-x}Sr_xVO_3$. One particularly interesting finding of ours concerns the temperature evolution of the low energy excitation attributed to orbital excitations and present in the insulating part of the phase diagram of $La_{1-x}Sr_xVO_3$ (near x=0) as well as in the closely related compound YVO_3 [4]. We performed a high resolution RIXS experiment studying the temperature dependence of this excitation and, using the temperature and doping dependencies of the energy of the excitation, we were able to unambiguously connect it to the antiferromagnetic and orbital ordering phase transition occurring in the $La_{1-x}Sr_xVO_3$ family of compounds at 140 K [5].

These initial findings, facilitated by the funding granted by Labex Palm, are leading into several manuscripts and allowed us to initiate a fruitful collaboration between the different groups involved in this project in order to develop a predictive ab-initio theory for RIXS as well as for a quantitative interpretation of the RIXS spectra.



Temperature and doping dependence of the observed low energy excitation in $La_{1-x}Sr_xVO_3$ for x=0 and x=0.1. The critical temperature of the antiferromagnetic and orbital ordering transitions is approximately 140 K. The sudden change in the temperature dependence of the energy of the excitation near the critical temperature connects the excitation to this phase transition.

K. Ruotsalainen, M. Gatti, J. Ablett, J.-P. Rueff, D. Adrian, W. Prellier and A. Nicolaou, *Low-energy electronic excitations and band-gap renormalization in CuO*, Physical Review B, 95, 19, 195142 (2017)

Résultats obtenus dans le cadre du projet MITRIXS financé par le thème 1 du LabEx PALM et porté par Alessandro Nicolaou (Synchrotron SOLEIL)