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Dynamics of transition metal cyanides with anomalous thermal expansion behavior

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Transition metal (TM) cyanides are an exceptional class of framework materials exhibiting remarkable physico-chemical aspects in terms of: (i) photoluminescence, (ii) dimensionality, i.e. these systems can be of a 1-D, 2-D or 3-D nature, and (iii) disorder, they can be subject to different types of disorder; like a site disorder on the TM site and/or a disorder of the C≡N bond, as well as stacking disorder in the 2-D (layers) case or a slipping disorder in the 1-D (chains) case.

The main interest in these materials goes beyond the above mentioned properties to cover intriguing phenomena like negative linear compressibility and negative thermal expansion (NTE). In some typical cases of TM cyanides, NTE can be colossal and extending over a wide temperature range, making it quite interesting and attractive both on the fundamental level as well as on the practical side for relevant applications.

Thermal properties are intimately linked to phonons in crystalline materials. Therefore studying phonon dynamics helps to gain deeper insights into the dynamical mechanisms of TM cyanides exhibiting anomalous thermal properties. Inelastic neutron spectroscopy (INS) is an appropriate technique to study lattice dynamics of crystalline materials on the microscopic level, offering the perfect tool to cover dynamics on the targeted length and time scales.

The presentation will focus on highlighting the relationship between lattice dynamics and the observed anomalous thermal behaviour in some selected one- two- and three-dimensional TM cyanide structures, to explore the microscopic mechanisms at the origin of their intriguing thermal expansion properties, by using a combined approach of INS, underpinned by ab-initio phonon calculations. For the sake of complementarity, results using other techniques (PDF, NMR, {\it etc.}) will also be indicated as to highlight the synergistic aspect of structure and dynamics in these fascinating materials.

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