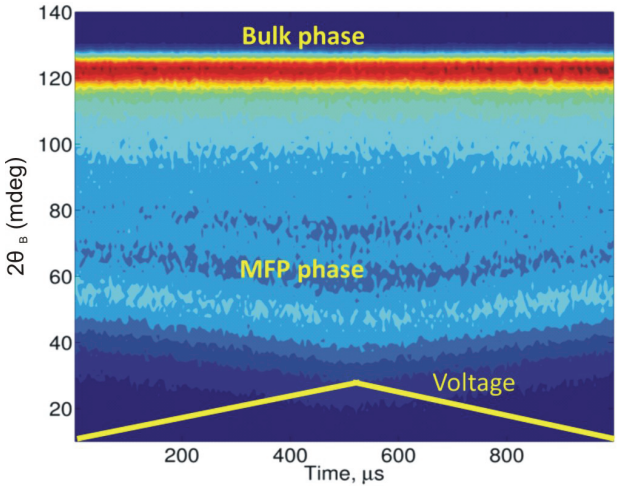

Figure 1. Time resolved X-ray diffraction 002 reflection under triangular shape 1 kHZ electric field (yellow curve). The top sharp peak corresponds to the bulk and deviated weak bottom peak corresponds to MFP phase

Keywords: time-resolved X-ray diffraction, SrTiO3, piezoelectricity

MS15-P29 Synthesis, crystal structure, spectroscopic characterization and theoretical study of Nicotinaldehyde N-phenylsemicarbazone

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Semicarbazones are derivative of imines compounds, which could be obtained by the condensation reaction between a ketones or aldehydes and semicarbazides. Semicarbazones exist in two tautomeric forms, keto (A) and enol (B) forms. The *keto* form acts as bidentate neutral ligand and the *enol* form can deprotonates acting as anionic ligand, making the semicarbazones versatile ligands in both neutral and anionic forms [1,2]. The coordination mode is influenced by the number and type of substituents groups; this is because the active donor sites of the ligand vary depending upon the substituents. In view of the importance of these compounds, the synthesis, crystal structure, spectroscopic characterization and theoretical study of Nicotinaldehyde N-phenylsemicarbazone have been carried out. In the first part of this study the semicarbazone molecule was synthesized and characterized by FT-IR, FT-Raman and NMR. The crystal structure was determined by X-ray single-crystal diffraction. The molecules crystallize in a $P2_1/c$ space group and form in the crystal packing N-H…O and N-H…N hydrogen bonds forming a centrosymmetric *synthon.* Other interactions like C-H…π and π…π stacking helps to stabilized the crystals. In the second part, the molecular geometry was optimized using DFT method and compared with the experimental data obtained from X-ray single-crystal experiment. The experimental (FT-IR) and calculated vibrational frequencies (using DFT) have been compared. The stability and charge delocalization was studied by natural bond orbital (NBO) analysis as well as the potential energy distribution (PED). Milliken population analysis on atomic charges is also calculated.

Acknowledments: Spanish Ministerio de Economía y Competitividad (MAT2013-40950-R) and ERDF funding is acknowledged.

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Keywords: Semicarbazone, single-crystal X-ray diffraction, DFT studies.