**Pressure-dependent modifications in the LaAuSb2 charge density wave system and differing pressure response of the structure in LaTMSb2 (TM = Au or Ag) ternary antimonides**

**Prof. Arumugam Sonachalam**

Vice Chancellor, Tamil Nadu Open University,

Centre for High Pressure Research, School of Physics, Bharathidasan University, Tamil Nadu, India.

**Abstract**

The effect of hydrostatic pressure on the LaAuSb2 charge density wave (CDW) system is studied using electrical transport, XRD, and density-functional theory (DFT). At 83 K, electrical transport data at ambient pressure show a clear CDW transition. With increasing pressure, the CDW transition shifts to a low temperature. Our resistivity data show that the CDW transition is completely suppressed at 3.6 GPa. At 3.8 GPa of pressure, the high-pressure XRD revealed a change from the linear trend for the out-of-plane (c) and the in-plane (a) lattice parameters. Further, a careful analysis of pressure dependence of several Bragg peak d-spacings revealed discontinuities on both the intensity and the full width of half maximum at around 3.6 GPa where the CDW transition is found to be fully suppressed from the electrical transport measurements. This reveals a clear link between the structural modulation and the CDW suppression in this system. Interestingly, DFT revealed a deviation in the c/a ratio around 8 GPa when compression was applied, together with weak anomalous behavior in the electronic band structure. From DFT the LaAuSb2 structure is found to be stable up to 150 GPa, however, a significant volume collapse is seen to occur around 100 GPa. Further, the ternary antimonides LaAuSb2 and LaAuSb2 share identical lattice symmetry and exhibit the CDW phenomenon. The CDW is found to be tunable either by physical or chemical pressure, triggering the investigation of the pressure response of these systems. Under hydrostatic pressure, the lattice structure of LaAgSb2 transformed from a tetragonal to a mixed tetragonal (4 GPa) followed by monoclinic (4–9 GPa) and then to a mixed monoclinic and orthorhombic (9–41.8 GPa) phases. In contrast, our synchrotron X-ray diffraction results on LaAuSb2 reveal that the tetragonal structure is stable in the pressure range of 0–12.2 GPa. Our experimental investigation is well supported by the DFT calculations. We have used DFT to identify the experimental Raman vibrational modes at ambient conditions. We highlight the importance of structural subtleties in the differing pressure response of the ternary antimonides.