➢ Static and Dynamical Properties of Perovskites (T, Bellaiche)

ABO_3 perovskites and related materials (such as hexagonal compounds and post-perovskites that share the same chemical formula) form important classes of materials that can display a wealth of phenomena, such as ferroelectricity, antiferroelectricity, magnetism, multiferroicity, charge and orbital orderings, and superconductivity. Consequently, they constitute a rich playground for research in physics, chemistry, engineering and material science, and are very promising to lead new technologies with phenomenal capabilities (e.g. actuators, sensors, memories, communication devices, ultrasound, and energy storage). There are three ways in which the tools and techniques of computational condensed matter can be used to understand these technologically important materials and to guide the development of the next generation of materials and devices: (1) provide solutions to complex phenomena that have been elusive for a long time; (2) design materials with optimized responses; and (3) discover novel phenomena of broad importance.

Students find the power and ability of computational methods to predict and understand material properties exciting and intriguing. Previous involvements of undergraduate students on different aspects of all three of the aforementioned research projects have led to exciting preliminary results. Undergraduate students can participate in several projects, where, in addition to state-of-the-art first-principles calculations, the following *ab-initio* numerical tools having unprecedented capabilities will be used: (i) effective Hamiltonian approaches that extend the reach of first-principles calculations by realistically mimicking properties of complex materials *at finite temperature and/or in the GHz-THz frequency range*; and (ii) the inverse method that allows an efficient design of materials with improved properties. Note that conventional numerical methods proceed by first specifying structural features of a given configuration (such as the locations of the different kinds of atoms in a solid solution), and then by calculating its properties. One can then change "by hand" these structural features in the hope of finding enhanced properties. Obviously, the inverse approaches - that consist in determining the crystal structure yielding pre-assigned properties --- are much more appropriate and efficient than conventional methods to predict real optimized materials.