Flexoelectric properties of bulk and 2D materials

Flexoelectricity - electromechanical coupling between mechanical strain gradient and electric polarization is a universal phenomenon. The flexoelectric effect is generally hard to detect in bulk systems but becomes significant in two-dimensional (2D) materials due to exceptional mechanical flexibility and the possibility of extremely large strain gradients. In this project by using state-of-the-art methods the students will develop a modeling framework that captures the influence of non-homogenous strain gradients on piezo, and flexoelectric properties. By studying flexoelectricity in various classes of bulk and 2D materials particular attention will be paid to finding the intrinsic features that dictate flexoelectricity of a material. These features will be used to identify good flexoelectric materials by scanning existing materials databases. These projects require that the student has basic knowledge of python and density functional theory. Student can choose one of the following options to purse this project.

Option 1: To develop a generalized phenomenological Landau model of polarization with strain gradients using inputs from density functional theory. This model will be very useful in developing a quick understanding of variation of polarization due to various type of strain gradient which are commonly found in 2D materials.

Option 2: Other possible option is to use density functional theory code to study flexoelectricity. In this project, the student will approach flexoelectricity for electronic structure calculations from a theoretical perspective and apply density functional perturbation theory to a prototypical material. This project involves the use of the open-source software Abinit on supercomputers. A prior basic knowledge of Linux and bash scripting is recommended.