Numerical Determination of Polar Surfaces

A Math 199 project, supervised by Christian Ratsch

For many devices in material science applications, surfaces are of particular importance. A surface is formed when a material is cut (along any of its directions). For crystalline materials, the detailed atomic structure of the surface depends on the direction of the cut. This is formally described by the so-called Miller indices. Now imagine that you have a piece of materials with multiple surfaces. For simplicity, let's consider a cube. A cube has 6 surfaces, with 3 sets of 2 surfaces that are parallel to each other. For further simplicity, let's consider only the top and bottom surface of this cube. For many materials, the detailed atomic structure of the top and bottom surfaces are identical (and there exists, for example, an inversion symmetry through the center of the cube). Such surfaces are called non-polar surfaces. But for certain orientations and certain materials, the atomic details of the top and bottom surfaces are different, no matter how you slice it (literally). These surfaces are called polar surfaces. Whether a surface is polar or non-polar has important implications. For example, for polar surfaces, one can never have a material where the top and bottom are microscopically the same, and thus they have different optical, electronic, or other properties.

It is the goal of this project to write an algorithm that determines whether the two surfaces of a given material are polar or non-polar. The material system is defined by the x-, y-, and z-coordinates of all atoms in the crystal, and the atom type. The first and easiest approach will be to calculate the distance matrices for all atoms on the top and bottom surfaces, and to compare these distance matrices. In principle, this is straightforward. But some technical details need to be dealt with; in particular, one needs to consider not just the given surface, but also translations (and maybe rotations), of the surface. Depending on the results and progress of this step, the student might also consider other approaches that make more explicit use of group theoretical and symmetry arguments.

The ideal student for this project is an applied math major with an interest in materials sciences. Applicants should be junior and senior with a GPA of 3.5 or higher, and should have strong computational skills. If you are interested, please contact Christian Ratsch by October 13: cratsch@math.ucla.edu.