

Surface vibrational modes in Bi₂Se₃, a layered topological insulator.

Topological insulators are a newly-discovered class of materials that are insulating in the bulk but have conducting surface electronic states that are required to exist because of certain topological characteristics of the bulk electronic bands. Besides their exotic electronic properties, several of these materials are also important for thermoelectric applications.

This project would require analysis of interatomic forces in Bi₂Se₃ (calculated using density functional theory) for structures with a varying number of atomic layers. Extrapolating from these calculations, a numerical model for vibrations in a semi-infinite bulk will then be defined and the normal modes of vibration of this system calculated. The modes will be examined to identify modes that may be confined near the surface. If time permits, the coupling of surface vibrational modes to surface electronic states will also be calculated and the time-variation of the electronic state energies following photo-excitation will be simulated and compared with time-resolved photoemission experiments. Most of the analysis will be computational and will require writing some new computer codes, as well as use of existing codes.

Supervised by: Stephen Fahy, Ivana Savic and Jose Querales in the Tyndall Materials Theory Group