In this talk, we will talk about some electronic structure study making use of algebraic theory. Density functional theory (DFT) has become a basic tool for the study of electronic structure of matter, in which the Hohenberg-Kohn theorem plays a fundamental role in the development of DFT. Unfortunately, the existing proofs are incomplete. In the first part of this talk, we shall present a rigorous proof for the Hohenberg-Kohn theorem for Coulomb type systems using the Fundamental Theorem of Algebra. Kohn-Sham equation, a nonlinear eigenvalue problem, is the most widely used DFT model. In the second part, after using group theory to divide an eigenvalue problem into some groups of smaller ones that can be solved independently and two-levely, we then apply the decomposition approach to electronic structure calculations of symmetric cluster systems, in which we solve successfully thousands of Kohn-Sham eigenpairs with millions of DOFs.

Graduate Students are encouraged to attend.