***Density Functional Theory: Short Basics and General Applications***

**Abstract**

Density functional theory simulation has risen as an important tool in the field of chemical engineering. DFT can access to a variety of atomic-scale properties and chemistry of materials that is difficult to be analyzed with easy-to-access characterization tools (such as XRD, NMR, IR, TEM, and SEM). DFT can, therefore, provide us to acquire useful information to support experimental observation as well as work as a bridge between experiment and theory. In this seminar, we will explore brief basics to understand what DFT is, how we can implement DFT into our research with several examples, and what DFT can do and cannot. The name, Density Functional Theory, is originated from its mathematical technique that employs electron density function rather than traditional electron wave function to solve the well-known Schrödinger equation. Such technique greatly reduces the scale of a calculation from a 3N-dimensional problem (N is the number of electrons) into a 3-dimensional problem. Accordingly, the development of DFT method allows us to simulate sufficiently large systems of interest (up to several hundred atoms and few nanometer scales) with modern computers. Then, we will explore practical applications of DFT, ranging from material science to (electro)chemistry, to understand how we can use DFT in our research and what DFT can and cannot do.