## Foundations of Density Functional Theory

N. V. Suresh Kumar
Assistant Professor of Physics
Department of Humanities and Sciences
VNR Vignana Jyothi Institute of Engineering and Technology, Bachupally, Nizampet,
Hyderabad, India - 500090

Computational methods of electronic structure theory are powerful techniques for predicting structure and properties of molecules and materials. Understanding the mathematical formulation of methods enables the user to evaluate results obtained from the methods. The presentation highlights basics of density functional theory (DFT), the prominently used method in molecular modelling. Also, tools for implementation of the method will be discussed.