Density Functional Theory for Nuclear Materials

NE XXX

1. **Course Overview**

In this course we will study the

XXXX

1. **Learning Outcomes**

By the end of this course, the student should be able to:

1. XXXXX
2. **Pre- or Co-Requisites**

NE 201

1. **Required Text(s)**

None.

Supplemental texts:

Light Water Reactor Materials, Vol. 1 Fundamentals, D. Olander and A. Motta

Nuclear Fuel Elements, B. Frost

Fundamentals of Radiation Materials Science, G. Was

1. **Course Requirements**

Examinations: Exam 1: 20 %; Exam 2: 20 %, Exam 3: 20 %

Projects: Presentation report 1: 10 %; Presentation report 2: 10 %; MOOSE Project 20%

1. **Topical Outline:** 
   1. Introduction and Overview
   2. Density Functional Theory Overview
   3. Electronic Optimization
   4. Ionic Optimization
   5. Special Quasi-Random Structures
   6. Ab intio Molecular Dynamics
   7. Quantum Espresso Overview (or abinit)
2. **Grading**

Letter Grade Percent Grade

A+ 98-100; A 93-97; A- 90-92; B+ 87-89; B 83-87; B- 80-82; C+ 77-79; C 73-76; C- 70-72; D+ 67-69; D 63-66; D- 60-62; F Below 60