

Homework 5

Designing a Lattice Visualization Tool Using Classes in Python

Student SB, HD, TS
Professor Jeffrey Carruthers
Release Date Oct 29 2024
Due date Nov 5 2024

Objective

Develop a Python program that models and visualizes crystal lattice structures using object-oriented programming principles. The assignment will focus on using Python classes, and optionally, inheritance, to represent atomic arrangements in simple cubic, body-centered cubic, face-centered cubic, and hexagonal close-packed structures.

Background Information

Each lattice structure has a unique arrangement and density, impacting its physical properties.

Simple Cubic (sc): Basic structure with atoms at each corner of a cube.

Body-Centered Cubic (bcc): Adds an additional atom at the center of the cube.

Face-Centered Cubic (fcc): Places additional atoms at each face of the cube.

Hexagonal Close-Packed (hcp): A non-cubic structure with a hexagonal pattern, known for high packing efficiency.

Include references to materials on atomic structures or crystallography to better understand these formations.

Deliverables

This homework's deliverables includes: Python code (.py or .ipynb)

Usage instruction files, background details and references (pdf or README file)

All files are to be submitted on Blackboard

Grading Rubrics

Class Structure Initialization (20 points): Correct setup of lattice attributes and structure handling. Method Implementation (30 points): Accurate implementation of plot lattice and supercell methods. User Interface and Usability (15 points): Well-defined interface, with clear prompts and error handling. Visualization Accuracy (20 points): Correct representation of lattice structures and supercells in 3D plots. Documentation Comments (15 points): Clear code comments, README file, and, if applicable, report documentation. Autograding Requirements provide examples of "how to use" the submitted software