

Short Course

Mineral Physics: Modeling from the Atomic to the Global Scale

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Geology was founded on the central insight that Earth materials are the products of planetary processes, the nature of which can be inferred by examining the rocks. But these processes are in turn governed by the physics and chemistry of the materials themselves, a way of thinking about Earth materials that came much later in the history of geology. There is a growing awareness that in-depth understanding of the physics and chemistry of natural materials can illuminate the origin and evolution of planets.

In this short course, we will view natural materials not only as the end products of geological processes, but as controlling those processes via their structure- and composition-specific behavior. The central conceit of building a terrestrial planet atom by atom, a coherent view of material behavior from the microscopic to the macroscopic, is approached via an overview of the phase equilibria of the deep Earth, the physical properties of its constituent phases, and frontier challenges in relating atomic structure and bonding to physical properties. Practical exercises give students hands on experience with cutting edge codes in mantle thermodynamical modeling and quantum mechanical simulation, and an opportunity to explore new frontier research directions.

Lectures

Mineralogy and petrology of Earth's Interior

Day 1 1st hour: Composition and structure of Earth's interior
Day 1 2nd hour: Mineralogy and crystal chemistry
Day 2 1st hour: Introduction to thermodynamics

Physical properties of earth materials

Day 2 2nd hour: Elasticity and equation of state
Day 3 1st hour: Lattice dynamics and statistical mechanics
Day 3 2nd hour: Transport properties

Frontiers

Day 4 1st hour: Melts and Fluids
Day 4 2nd hour: Electronic structure and ab initio theory
Day 5 1st hour: Building a terrestrial planet

Practicals

Day 1: Constructing Earth models: Thermodynamic modeling

Day 2: First principles computation of physical properties: Quantum mechanical simulation

Remaining Days. Student-driven research projects based on computational tools used in first two practicals.