

CENTER FOR COMPUTATIONAL SCIENCES (CCS)/CENTER FOR ADVANCED VEHICULAR
SYSTEMS (CAVS), MISSISSIPPI STATE UNIVERSITY

JOINT FORUM ON MATERIALS SCIENCE

(Academic year '06 - '07)

CCS and CAVS will host a joint forum on materials science throughout the academic year '06-'07. In the fall of 2006, biweekly lectures by mathematicians, physicists, and engineers will be organized. In Spring 2007, we will host a colloquium series in materials science.

Density Functional Theory in Materials Science

DR. SEONG-GON KIM

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Dates: Lecture 3 - Friday, October 13, 2006

Lecture 4 - Monday, November 20, 2006

Time: 3:00 - 4:00 p.m.

Location: CAVS SEMINAR ROOM

Abstract. Modern materials science increasingly demands the understanding of phenomena that determine properties of materials on an atomistic level. The interaction between atoms and electrons are governed by the laws of quantum mechanics; hence basic knowledge in quantum mechanics is essential to all practitioners of materials engineering. Density Functional Theory (DFT) represents one of the most important breakthroughs in computational techniques for solving fundamental quantum-mechanical equations for complex many-atom, many-electron systems relevant to materials science. In these two lectures, I will review the fundamental principles of quantum mechanics most relevant to materials engineering. I will also introduce the basic principles of DFT and its applications in materials science.

There will be a refreshment between 2:45 - 3:00 p.m. each day in the CAVS SEMINAR ROOM.

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