

総合科学技術共同教育センター (GJEC) 集中講義のご案内

総合科学技術共同教育センター(GJEC)・国際共同教育部門では、海外から客員教授を招聘し、集中講義を行っています。今回は、チェコより Mojmir Sob 先生(Academy of Sciences of the Czech Rep) をお呼びし、下記のとおり集中講義を行います。

Announcement of Lectures in English (Professional Education)

Global Joint Education Center for Science and Technology (GJEC) will offer the following intensive course in English. Advanced Science and Technology C-6

Title: **Ab Initio Electronic Structure Calculations in Multiscale Modeling of Materials**

Instructor: **Prof. Mojmir Šob** (Academy of Sciences of the Czech Rep.)

Credit: 1 credit Code: (Master) 39926 (Doctor) 69926

Schedule:

September 26 (Mon) 10:00 - 12:00

September 27 (Tue) 9:00 - 12:00

September 28 (Wed) 9:00 - 12:00

September 29 (Thu) 13:00 - 16:30

September 30 (Fri) 13:00 - 16:30

Place: Room308 Faculty of Engineering Research Building I

Category: III (Text: English, Speaking Language: English)

Abstract: Basic of ab initio approach to electronic structure of solids. Schrödinger equation for a solid, Born-Oppenheimer approximation, density functional theory, functional of the exchange-correlation energy, its local approximation. Principle of methods of electronic structure calculations and their survey (APW, OPW, LCAO, KKR, LMTO, LAPW, pseudopotentials, KKR). Bloch theorem, tight-binding approximation. The role of Green functions in solid-state theory, expression of local density of states and of charge density in terms of Green functions. Electronic band structure of metallic materials, density of states, structures with higher energies, polymorphism of metals. Magnetism of solids, its origin, description of electronic states, Heisenberg and Stoner model of magnetism. A review of basic types of magnetic behavior (dia-, para-, ferro- and antiferromagnetism). The importance of total energy for studies of stability and

properties of materials, existence of structures with higher energies and polymorphism, modelling of configurations of extended defects, theoretical strength of materials. Multiscale modelling: from electronic and atomic dimensions through mesoscopic level to continuum.

Add and Drop: If you would like to register/cancel classes, submit an Add/Drop form at Project Support Section during registration/cancellation period below.

Registration period: August 22 (Mon.) to September 16 (Fri.)

Cancellation period: August 22 (Mon.) to September 29 (Thu.)

Note: Make sure to submit the form if you do not intend to attend a class after the registration. Otherwise your grades are processed as registered.

Note: Both Master's and Doctoral students can take the class. Students who enrolled before April 2009 can audit but not earn a credit. Inquiry and registration: Project Support Section (1F, Faculty of Engineering Bldg. No.1) szk-project@jimu.kumamoto-u.ac.jp