International Conference on Advanced Materials (ICAM-2011)
International Workshop on Computational Materials Science
Using Full-potential Methods
December 12-16, 2011
Department of Physics, PSG College of Technology, Coimbatore - 641 004
Tamil Nadu, India

Conveners
Dr. Olle Eriksson
Uppsala University, Sweden
Dr. P. Ravindran
University of Oslo, Norway
Dr. S. Jayakumar
PSG College of Technology, India

Scientific Objectives
The workshop has the following objectives:

- Training beginners of electronic structure theory using Full-potential basis functions in the RPW and ELK implementations.
- Discuss recent developments at theoretical level beyond LDA, TDDFT, DMFT, excited states as well as software level (e.g., parallelization, interfacing with other codes / modules, plans for future implementations).
- Communicating most recent scientific achievements and results obtained by the FP-LMTO-REVPP and FP-LAPW-ELK schemes.

Description
The workshop will cover the fundamentals of modern electronic-structure methods based on density functional theory, with emphasis on the Full-potential Linear Multi-Elemental Orbital (FMLMTO) method and Full-potential Linearised Augmented Plane Wave (FLAPW) method, together with some of the most recent developments and applications. The present workshop focuses on covering theoretical, practical, and numerical aspects of LDA+/DMFT and LDA+/Hubbard U, LSCO, La2-xSrxCuO4, GDFT, GW, GGA+U, Coulomb interactions, Linear and Non-linear optics, BESS, and level optimization.

The activity will be divided into three parts:

1. A basic introduction to computational materials theory based on density functional methods with emphasis on recent developments of electronic structure methods in materials science and their implementation in REVPP and ELK codes.
2. Advanced sessions highlighting applications of new developments of electronic structure methods for advanced materials relevant to emerging technologies.
3. Experts and developers from 12 different countries shall deliver special lectures.

4. Hands-on computer sessions based on the REVPP FMLMTO and ELK FLAPW codes.

On the basis of our previous experience with the organization of workshops Jat Sanders, Elswit, Uppsala, Sweden, 33...Ljusarne, see http://www.rpsost.org and http://elk.sourceforge.net, the presentation of the theory will be followed by practical exercises and hands-on tutorials. The participants are expected to have background knowledge in Condensed Matter Physics and/or Solid State Chemistry. Some knowledge of using Linux will be an advantage. The participants are expected to have a fair knowledge of DFT prior to the workshop (see Refs). Although at the beginning of the school, we will make sure that the DFT level of all participants is enough in this respect and provide the needed complementary information and training; the purpose of the school is to go beyond DFT with hands-on exercises based on full-potential implementations.

The workshop is meant to be a genuine forum of interacting experts-novices in order to increase efficiency and outreach of the FMLMTO-REVPP and FLAPW-ELK apparatus. It is an expert-teacher- and training-place for developers and young researchers by an uncommonly interactive, self-supervised, and open level of communication among all participants. At the end of the workshop, students will have sufficient working experience to pursue their projects at their home institution.

References

Registration
Registration form can be downloaded from the conference website: www.psychistech.in/ICAM2011. Registration fee will be paid in the form of demand draft drawn in favour of ‘The Principal, PSG College of Technology’ payable at Coimbatore.

REGISTRATION CATEGORY

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Academics: Rs 4500; Industry: Rs 7000; Students: Rs 4500; Participants from abroad: Rs 5500.

*Registration fee is subject to only limited number of participants on first come first serve basis.

For further details and information contact:
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