Graduate Course on
Ab initio Modelling of Solar Cell Materials

Credits : 5 points

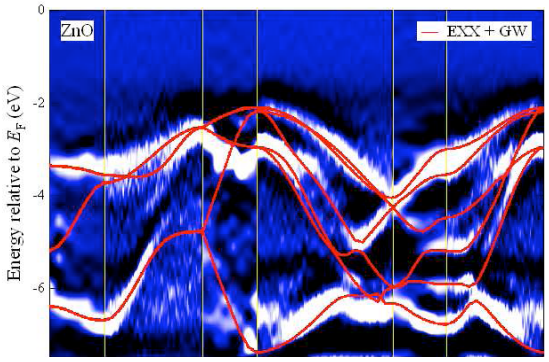
Spring 2010

Course Starts Monday, 15 March 2010

Dr. P. Ravindran, University of Oslo

To register the course send email to : ravi@kjemi.uio.no

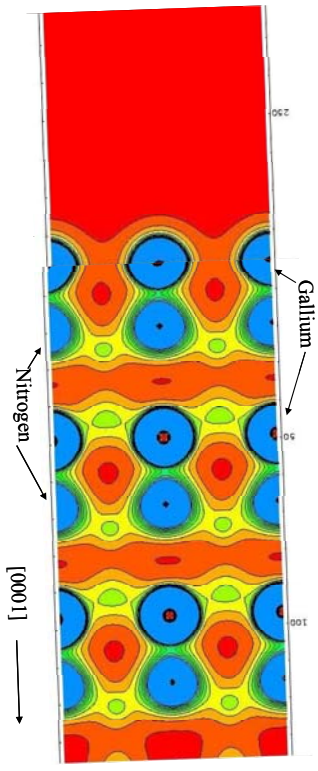
What is the course about?



Week 11 **Part I. Electronic structure – Basic Theory & Application to Solar Cell Materials**

- **Density Functional Theory**
- **Functionals for Exchange and Correlation**
- **Electronic structure methodology – LMTO, LAPW and PAW methods**
- **Electronic band structure & DOS related properties.**
- **Hands on training with abinitio codes to simulate absorbers, electrodes, TCOs and antireflection coating materials.**

Week 15 **Part II Simulation of Advanced Properties of Solar Cell Materials based on DFT.**



- **Simulation of Defects**
- **Optical Property studies**
- **Simulation of Thinfilms & Nanophases**
- **Hand on training with ab-initio codes to simulate Advanced Properties of Solar Cell Materials**

Literature: Richard. M. Martin, Electronic Structure:Basic Theory and Practical Methods. & Lecture Notes.

Practical Information:
Homepage: http://folk.uio.no/ravi/FME-SOL
Lectures: First lecture starts Monday 09.00 15 March 2010 at V172 in Kjemisk Institute, University of Oslo, Blindern.

Possible projects:

1. Theoretical study of optical properties of solar cell materials
2. Modeling of nanophases/thin films of solar cell materials
3. Simulation of defects in semiconductors

Evaluation:

- Computational Exercises
- Project report (should be delivered one month after the completion of teaching).