Program Schedule for School Part-1
(6-th -9-th Jan, 2014)

	9:00-10:30	10:30-11:00	11:00-12:30	12:30-14:00	14:00-15:30	15:30-1600	16:00-17:30	17:30-18:30
Mon. 6-th Jan.	Blaha	Coffee	Harbola	Lunch	Harbola	Coffee	Marzari (Skype)	Q/A session
Tues. 7-th Jan	Vanderbilt (Skype)	Coffee	Blaha	Lunch	Shenoy	Coffee	Tut. on WIEN2K	Tut. on WIEN2K
Wed. 8-th Jan	Sarma	Coffee	Shenoy	Lunch	Aryasetiwan	Coffee	Tut on WIEN2K	Tut. On WIEN2K
Thurs. 9-th Jan	Shenoy	Coffee	Aryasetiwan	Lunch	Aichhorn	Coffee	Tremblay	

Details of the Lectures during the School Period

1. M. Harbola (IIT Kanpur, India)

An Introduction to Density Functional Theory

2. P. Blaha (Technical University, Vienna Austria)

a) **Basic concepts of bandstructure methods and the APW based methods**
(Contain a general discussion of the underlying concepts and a description of the development from Slaters original APW method to the modern APW+lo method).
References:
i) D.Singh and L.Nordstrom: Plane waves, pseudopotentials and the LAPW method, 2nd ed. Springer, New York 2006
ii) G.K.H.Madsen et al., Phys.Rev B 64, 195134 (2001)
iii) C.Ambrosch-Draxl and J.Sofo, Comp.Phys.Commun. 175, 1 (2006)
iv) D.Koelling and B.Harmon, J.Phys.C: Sol.St.Phys., 10, 3107 (1977)
v) J.Kunes et al., Phys. Rev. B 64, 153102 (2001)

b) **WIEN2k: methods and features (http://www.wien2k.at/)**
(Contain a discussion of advanced topics like structure optimization, spin-orbit coupling, various spectroscopies)

c) **Tutorial on WIEN2k**
The tutorial on wien2k would give first a short introduction into the code, but then mainly a live demonstration how to run calculations with WIEN2k.

3. D Vanderbilt (Rutgers University) and N Marzari (Lausanne)

a) Wannier Functions: Theory and Practise

The theory of Wannier functions for both isolated and entangled bands; projection vs localisation; practical construction of Wannier functions

b) Wannier Functions: Model Hamiltonians and Interpolation

Wannier functions as a minimal basis, interpolation of k-space properties, calculation of properties such as Berry Curvature, electronic transport

Ref: Maximally localized Wannier functions: Theory and applications Rev. Mod. Phys. 84, 1419-1475 (2012)

http://www.wannier.org/

4. Vijay Shenoy (IISc. Bangalore, India)

Review of many body field theory

Include Green function and response functions, saddle point analysis.
These ideas will be illustrated in the Anderson impurity problem.

5. D.D. Sarma (IISc Bangalore)

Correlations and spectroscopy

6. F. Aryasetiwan (Lund University, Sweden)

First-principles method for calculating the Hubbard U (I & II):

The Hubbard model
Herring's definition of U
Constrained LDA (cLDA)
Coulomb screening in solids
Linear response function
The random-phase approximation (RPA)
Constrained RPA (cRPA)
Wannier orbitals
cRPA for entangled bands
Applications of cRPA
Connection between cLDA and cRPA

References:
cLDA: Gunnarsson *et al* PRB 39, 1708 (1989)
cRPA: PRB 70, 195104 (2004)

7. André-Marie Tremblay (Universite de Sherbrooke , Canada)

Title: High-temperature superconductors: Where is the mystery?

Abstract: High-temperature superconductors belong to the class of materials which has probably been subject to the largest number of experimental enquiries in the last 25 years. This talk will review some of the important results of these investigations, contrasting the hole- and electron-doped cases. The evidence for Mott physics and for phase competition will be discussed along with the relevance of the one-band Hubbard model.