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

<table>
<thead>
<tr>
<th>Time</th>
<th>Mon. 6-th Jan.</th>
<th>Tues. 7-th Jan</th>
<th>Wed. 8-th Jan</th>
<th>Thurs. 9-th Jan</th>
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</thead>
<tbody>
<tr>
<td>9:00-10:30</td>
<td>Blaha</td>
<td>Vanderbilt (Skype)</td>
<td>Sarma</td>
<td>Shenoy</td>
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<tr>
<td>10:30-11:00</td>
<td>Coffee</td>
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<td>11:00-12:30</td>
<td>Harbola</td>
<td>Blaha</td>
<td>Shenoy</td>
<td>Aryasetiwan</td>
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<td>12:30-14:00</td>
<td>Lunch</td>
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<td>14:00-15:30</td>
<td>Harbola</td>
<td>Shenoy</td>
<td>Aryasetiwan</td>
<td>Aichhorn</td>
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<tr>
<td>15:30-1600</td>
<td>Coffee</td>
<td>Coffee</td>
<td>Coffee</td>
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<tr>
<td>16:00-17:30</td>
<td>Marzari (Skype)</td>
<td>Tut. on WIEN2K</td>
<td>Tut on WIEN2K</td>
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<td>17:30-18:30</td>
<td>Q/A session</td>
<td>Tut. on WIEN2K</td>
<td>Tut. On WIEN2K</td>
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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 Slatners original APW method to the modern APW+lo method).

   References:

   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


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:
   cRPA: PRB 70, 195104 (2004)

7. **André-Marie Tremblay** (Université 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.