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Computational Aspects of Materials Science

22 JUN 2018 @ PRASANTHI NILAYAM CAMPUS

Department of **PHYSICS**

The Department of Physics, SSSIHL organized a one-day workshop on the **Computational Aspects of Materials Science**.

The workshop provided students with the theoretical basis of **Density Functional Theory (DFT)** and a quick hands-on exposure to **Quantum Espresso** software.

Dr. R Gowrishankar, Head, Department of Physics, welcomed the participants and spoke on the purpose of the workshop. He highlighted the usefulness of the doing computational studies to understand materials properties. He then went on to introduce the speaker of the day, **Sri Mit Naik**, an SSSIHL alumnus who is currently a Doctoral Research Scholar at Indian Institute of Science, Bangalore.

During the morning session, Sri Naik introduced the Density Functional Theory along with the techniques employed by Quantum Espresso in modeling and studying material properties.

The afternoon session was dedicated to getting a quick exposure to using the software **Quantum Espresso**. The participants learnt how to create input files with specific parameters that are used as input for calculations. Band structures of a few known materials were studied as examples.