

A joint ASET-Vigyan Vidushi 2024 (Physics) Colloquium

Bibha Chowdhury Memorial lecture



Why do Computations? Designing Novel Materials from First Principles

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Materials play such an important role in human lives, that progress in human civilization is labeled by the materials used in that era (the Stone Age, the Bronze Age, etc.) Throughout most of history, new materials were discovered either by accident, or by a process of trial and error. However, nowadays, we wish to instead carry out a process of rational design. In this endeavour, density functional theory calculations (also called first principles calculations) play a vital role. I will give a simple introduction to this field, with a few examples of research from my group over the years. I will try to convince you that the field has now advanced to a stage where it can predict new materials that can be experimentally synthesized, as well as provide theoretical insight into experimental observations. This saves both time and money!

Shobhana Narasimhan got her MSc from IIT Bombay in 1985 (with an Institute Silver Medal) and Ph.D. from the Harvard University in 1991. After postdocs at Brookhaven National Laboratory, USA, and the Fritz Haber Institut, Berlin, Germany, she joined the faculty of JNCASR, Bengaluru, where she is a Professor in the Theoretical Sciences Unit. She is a Fellow of the Indian Academy of sciences and the National Academy of Sciences of India, and also of the American Physical Society and the American Academy of Arts and Sciences.

In addition to her research in computational nanoscience, she has a strong interest in promoting the cause of women in science, and in the teaching of physics in developing countries.



Time: May 31, 2024 at 4 pm

Venue: TIFR Colaba, Room AG66

YouTube link <https://youtu.be/a0ksPKIECU8>

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