



Satyendra Nath Bose
National Centre
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Bose Colloquium



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04:00 PM



Webinar Link



YouTube Link

Title:

Designing novel nanomaterials: one atom at a time

Abstract:

The development of new materials signals the progress of civilizations. Throughout history, novel materials were mostly identified either accidentally or through a process of trial and error. We now want to replace this by a program of rational materials design. In such an approach, computational calculations play a vital role. It is now possible, using density functional theory, to perform extremely accurate calculations, that can save considerable time and money. I will present an overview of the field, with examples from research in my group, in the areas of nanomagnetism, nanocatalysis and self-assembly.



Speaker

Prof. Shobhana Narasimhan

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