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Being a Little Bad: Defects in 2D Materials

As with bulk materials, defects can significantly alter the properties of a two-dimensional material. Defects can have a deleterious effect, or they can confer desirable properties that can be exploited for specific applications. I will give a review of experimental and theoretical work on defects in two-dimensional materials such as graphene and its successors. I will also discuss work in our group, where we have used density functional theory to study defects in twisted bilayer graphene and in few-layer phosphorene.

Shobhana Narasimhan is a Professor of Theoretical Sciences at the Jawaharlal Nehru Centre for Advanced Scientific Research in Bangalore, India. Her group works in the area of computational nanoscience. They use the techniques of density functional theory to understand the properties of nanosystems, and then use this knowledge to design novel nanomaterials with desired properties. Topics of recent interest include 2D materials, nanocatalysts, self assembled monolayers, spintronics and molecular machines.