



Physics Colloquium

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Properties and design of nanomaterials from first principles

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ABSTRACT

Nanomaterials, i.e., materials or structures that have at least one dimension between 1 and 100 nm, constitute the cornerstone of all modern materials science and technology and have revolutionized the design and functionalities of modern technological applications. However, due to the dimensions and complexity of these nanostructures, it is not always straightforward or even possible for experiment to identify the dominant mechanisms governing the properties of nanomaterials. However, in nanomaterials research, the role of Computational Materials goes beyond that of complementary to experiment: They provide insights into the scale of nanophysics and in synergy with experiment play a central role in the investigations and design of novel materials.

In the present talk I will focus on a common key characteristic of all nanomaterials, i.e., surfaces and interfaces, and demonstrate how first principles based calculations can boost the research and design of novel nanomaterials. Specifically, I will address how the interplay between quantum mechanics at surfaces, topology at interface junctions, and strain and chemistry, govern the growth and the properties of nanostructures. Furthermore, I will discuss how this information can be employed to understand and guide experiment as well as to design routes to grow alloys with properties that overcome limits imposed by bulk thermodynamics. To demonstrate these, I will use examples from the fields of III-Nitrides and multi- and poly-crystalline Silicon, i.e., materials of high technological interest for optoelectronics, powerelectronics and photovoltaic applications. Specifically, the topics of Nanowires^{1,2}, Quantum Wells^{3,4} and nanopines in binary and ternary III-Nitride alloys⁵ and interfaces⁶ and interfacial junctions⁷ in Silicon will be addressed in details.

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