INDO SWISS JOINT RESEARCH PROGRAMME (ISJRP)

JOINT RESEARCH PROJECT

ABSTRACT

Grant No.: 138871

DESIGNING NANOSTRUCTURES FOR NOVEL FUNCTIONALITIES

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Official start date of the project: 1st January 2012
Actual start date of the project: 1st April 2012
Project finish date: 31st March 2015

PROJECT ABSTRACT

The fact that the geometric structure of a molecular system determines all its physical properties, makes the determination of the structure the most important task in condensed matter research. There are umpteen instances of structurally different nanosize structures of the same material with drastically different properties. For a full understanding of these systems it is however not enough to find the ground state structure, but one has to explore the entire energy landscape of the system. Methods like minima hoping that give this information are therefore essential in the study of such nanosize structures. An understanding of the electronic structure and some of the observable properties like optical absorption, photoelectron spectroscopy and electrical conductivity can then guide the design and experimental realization of nanostructures with desired properties. The determination of the ground state and some of the metastable structures and their properties are the two complimentary aspects to be studied by the Basel and Pune groups respectively.

The control of the magnetic properties of semiconductor nanostructures poses problems. Moreover, device miniaturization does not reduce power consumption. Electric-field control of ferromagnetism in a diluted magnetic semiconductor, on the other hand, has been shown to be useful in scaling the microelectronics to the next generation of nanometre-sized integrated chips for low power consumption and low variability. However, these effects have not been related to structural changes due to applied electric field. We plan to include in our investigations low-lying structure that are very close in energy but are different structurally, and look among these for structures that can be obtained from each other by the application of an electric field. Stable cage-like structures and core-shell structures, with or without doping; have been of interest both from the understanding point of view and usefulness for specific applications. These structures can also be building blocks for self-assembly. In this project, we aim to find out such useful structures and understand their stability. We intend to study Fe@Au core shell structures which have potential applications in biomedicine and doped and undoped ZnS@CdS structures for possible optoelectronic device applications. We will also study some experimentally fabricated core shell structures where the shell consists of fairly large molecules whose arrangement cannot be determined experimentally.