



## INDO SWISS JOINT RESEARCH PROGRAMME (ISJRP)

### JOINT RESEARCH PROJECT

#### **ABSTRACT**

**Grant No.: 138856**

#### **LIGAND ENGINEERING FOR THE SURFACE MODIFICATION OF MOLECULAR SCALE AU NANOWIRES FOR BIOMEDICAL APPLICATIONS**

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#### **PROJECT ABSTRACT**

Nanoparticles, synthesized by wet chemical methods, are typically stabilized against aggregation by attaching molecular monolayers (ligands) to their surface. Since the interaction of the particles with the outside world is mediated through these ligands, this monolayer has a profound influence on many of the properties and applications of nanoparticles. Sensing, pseudo-enzymatic activity, directed assembly of particles to form supracrystals are a few striking examples where the ligands play a major role. While it is recognized that the ligand functional group is critical in determining individual/collective nanoparticle behaviour, the influence of ligand assembly/order on the particles' properties is often ignored. Recent studies of mono- and multiple ligand ordering on topologically spherical Au nanoparticles have clearly demonstrated that several properties of nanoparticles including wetting behaviour, interfacial energy, and cell-membrane penetration critically depend upon the nature of ligand order on the nanoparticles surface.

The problem of packing entities on a curved surface is relevant in a variety of fields including physics, biology and mathematics. When a mixture of ligands with different attributes (chain length, for instance) arrange on a nanoparticle surface, a range of ordered structures ranging from stripes to fully separated domains form depending on the ratio of chain lengths and the diameter of the particles. Since some of the properties of the particles (but probably also of the core) are dictated by the nature of order in the ligand shell, there is a strong motivation to understanding the role of various parameters on the ordering process. Such studies have been recently carried out for the case of multiple ligands on spherical Au surfaces, both experimentally and through simulations (molecular dynamics and coarse grain).

The primary motivation of the present proposal is to carry out detailed studies on the assembly of mono- and multiple ligands on cylindrical Au nanostructures as typified by nanowires and nanorods and to investigate the properties of such nanostructures. While the research group of one of the investigators (FS) has been carrying out extensive studies on the assembly of ligands on Au nanoparticles that are topologically equivalent to a sphere, the other investigator's group (NR) has developed a method for synthesizing molecular scale, single crystal Au nanowires (~ 2 nm in



diameter) that provides an ideal platform for carrying our fundamental studies on a truly one-dimensional (1D) system. The present proposal will investigate the assembly of ligands on these nanowires that are topologically equivalent to a cylinder. Ligand-exchange reactions will be carried out to replace the oleylamine capping on the nanowires. The structure and possible ordering of the ligands will be studied using STM-based techniques. A pronounced effect of the size of the particles on the nature of ordering of ligands has already been demonstrated for spherical nanoparticles. We propose to investigate Au nanorods with larger diameters to determine the role of nanoparticles dimensions on the nature of order of the ligand monolayers and compare it with theoretical predictions. Cell-membrane penetrating nanowires will be synthesized by engineering the ligands on the surface. Since the nanowires absorb in the near IR regions, this could, in principle be used for local heating if the nanowires could be directed towards tumour regions.