

**A Detailed description of the thesis proposed by Dr. Safi Jradi¹ and
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3D Hybrid Nanostructures for Ultra-sensitive chemical detection

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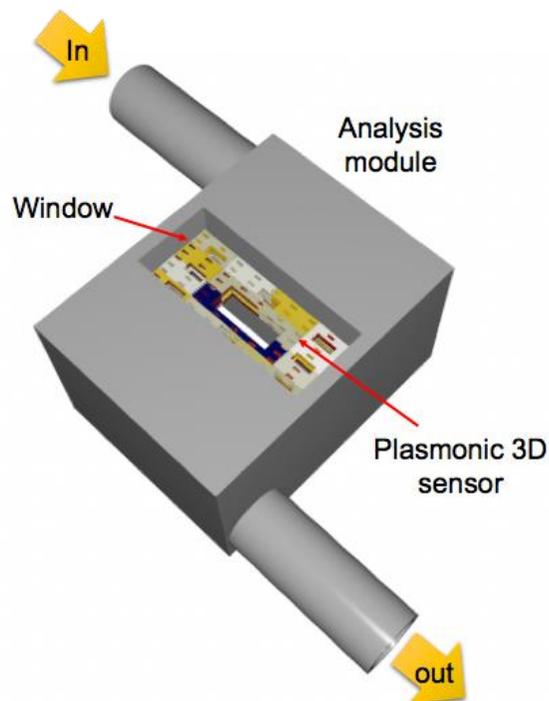
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Determining the chemical structure is crucial to many applications, and especially in medical diagnosis, environmental monitoring, and national security. Chemical sensing methods based on vibrational spectroscopy (IR or Raman spectroscopy) provide molecular "fingerprints" and are easy and fast to apply in the field to liquid, gas, or solid samples. The main issue is its low sensitivity. The most efficient method to improve it is the use of gold or silver nanoparticles that amplify the optical signal by several orders of magnitude. This method is known by Surface Enhanced Raman Spectroscopy (SERS). There are a lot of strategies to fabricate high sensitive SERS substrates allowing strong field enhancement and thus high SERS sensitivity, including e-beam lithography, chemical synthesis and assembly techniques. The aim of these strategies is to increase the local field enhancement as well as the interaction between the nanoparticles and the target molecules. In this context, one of the most promising approaches is to combine the 3D lithography technique with the chemical synthesis in order to assemble metallic nanoparticles with a high density of hot-spots (strong field enhancement).

The aim of the present PhD project that will be co-supervised by UTT and TPU is the fabrication of 3D hybrid nanostructures that provide extreme enhancement to the optical spectroscopy signals due to their unique 3D nanostructure. The proposed project combines three exciting research fields:

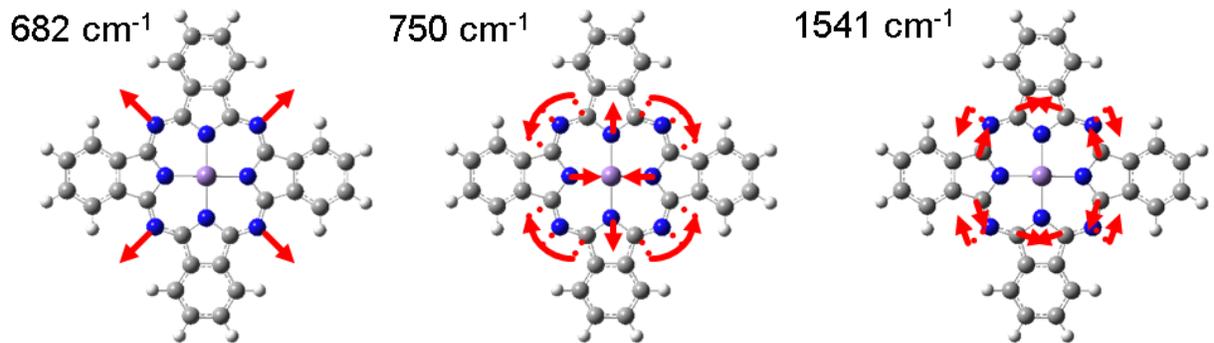
- (1) Chemical fingerprinting by optical spectroscopy
- (2) Signal enhancement by nano-optics and plasmonics
- (3) Fabrication of 3D-printed nanostructured polymer scaffolds

This combination will enable the ultra-sensitive detection of low molecular concentrations that can make an impact in environmental control, medical diagnosis, and national security applications. Below you will find the short description of each component.

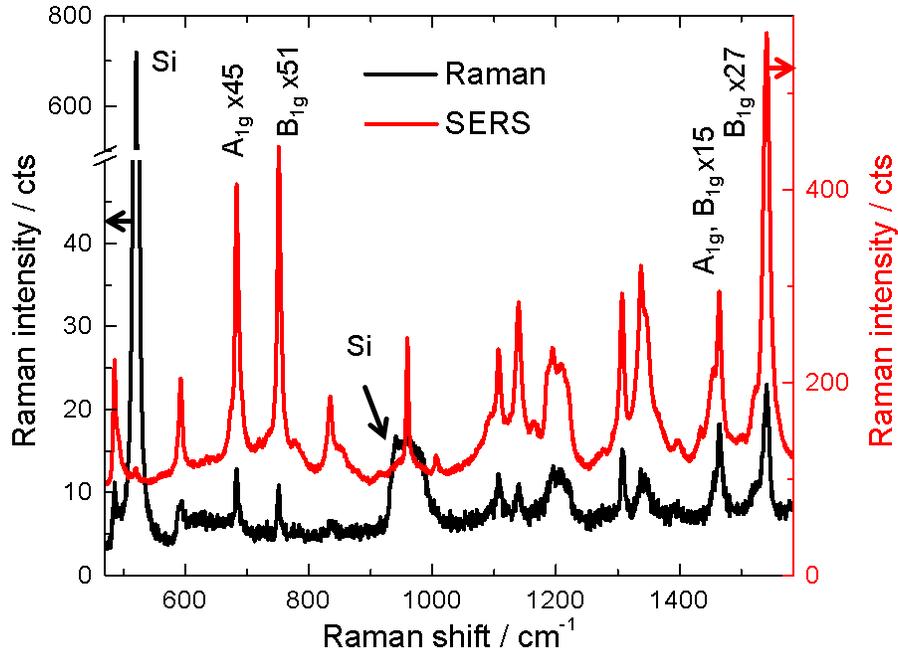


(1) Chemical fingerprinting by optical spectroscopy

Each molecule possesses vibrational frequencies that are determined by the mass of the atoms and the strength of the chemical bonds. As an example, below you can see three vibrations of cobalt phthalocyanine (CoPc) molecules and their frequencies in reciprocal cm (from DFT calculations, collaboration with Dr. Lehmann, TU Chemnitz, Germany).

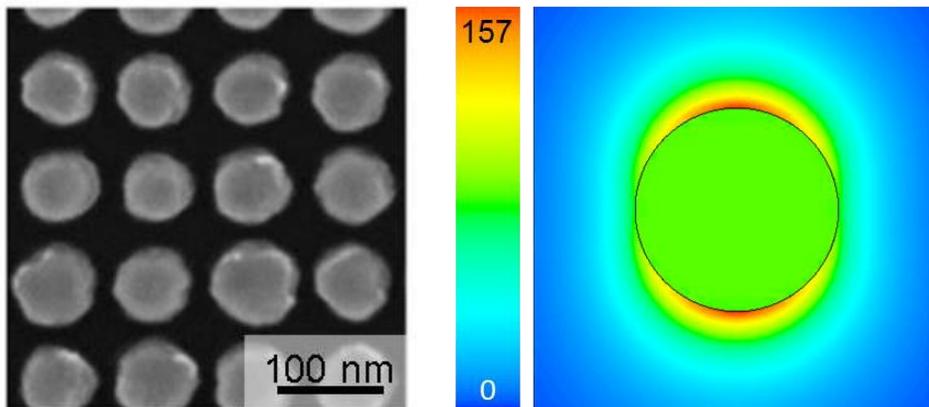


The set of frequencies, its "fingerprint", is specific to a molecule and can be used to identify it. The vibrational Raman spectrum of CoPc is shown below. The black curve is the standard Raman spectrum, and the red curve is the spectrum enhanced by plasmons in gold nanoparticles. SERS stands for surface-enhanced Raman spectroscopy. In this case, the signal enhancement is 30-fold, and the enhancement factor provided by the nanoparticles is 2000 times.



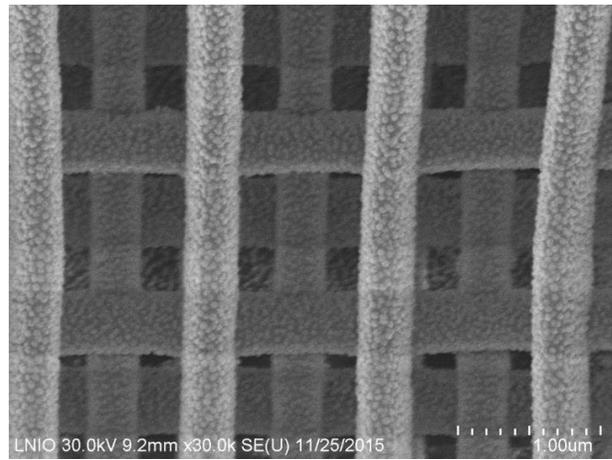
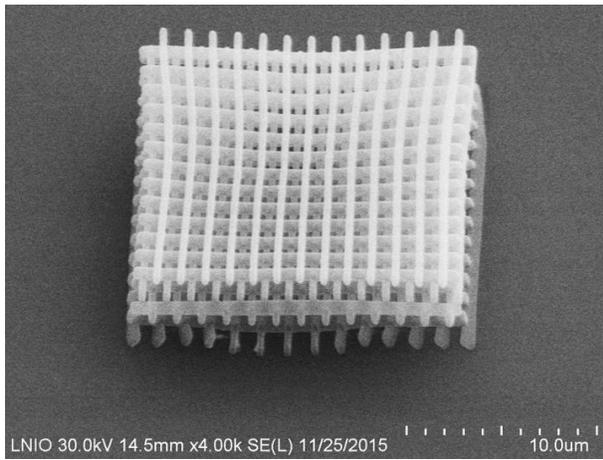
(2) Signal enhancement by plasmonic nanostructures

The sensitivity improvement can reach up to 1 billion times allowing the detection of a *single molecule*. This signal amplification is possible due to gold nanoparticles (left, gold nanoclusters prepared by electron beam lithography, by E. Rodyakina, ISP RAS, Novosibirsk, Russia) that strongly enhance the electric field (right, finite element methods simulations of 10 nm sphere with dielectric constant -2, collaboration with Dr. Kochuzhin).



(3) Fabrication of 3D-printed nanostructured polymer scaffolds

The goal of this research is integrating gold nanoparticles in 3D polymer scaffolds, like those shown below, and optimizing these nanostructures for the SERS detection of small concentrations of molecules. The scaffolds are fabricated by a two-photon polymerization technique that makes it possible to prepare 3D photonic nanostructures with specific optical properties.



The successful candidate will develop and apply unique 3D photonic polymer nanostructures covered by noble metal nanoparticles to enhance the optical spectroscopy signals for the applications in chemical and biosensing. The candidate will establish a technology to achieve high degrees of signal enhancement by optimizing the structure parameters to particular applications in medical diagnosis or national security and by integrating the structures in a 3D printed portable cuvette.

The PhD student will be in charge of the design, fabrication and characterization of 3D hybrid nanostructures. This part will be done in the Nanomat platform located at UTT and supervised by Dr. Safi Jradi. The second part of the PhD will be co-supervised by Prof. Evgeniya Sheremet at Tomsk Polytechnic University where the 3D hybrid nanostructures will be studied and characterized in SERS detection. The PhD student will stay at least 4 months/year at TPU. He/she will develop and test portable Raman cuvettes

integrating these 3D nanostructures for their application in liquid and gas sensing. He/she will be in charge also of the structural and optical characterizations of the resulting 3D hybrid structures.

The candidate should have good skills in at least one of the following topics: Materials Science, Nanomaterials, Plasmonics, Nanofabrication, Photopolymers. He/she should have good communication skills in English.

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