1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan, all in English)

Project title: Numerical model of single biomolecule detection in plasmonic nanoparticle ensembles

1.1 Project Goals

Label-free detection of single biomolecules relying on localized surface plasmon resonance (LSPR) sustained by metallic nanoparticles (NPs) could satisfy the rapidly growing need for fast and sensitive sensors in medical diagnostics. The current challenge is to increase the sensitivity and specificity of plasmonic biosensors to detect rarest species in small sample volume [1].

The proper understanding of the interactions between light and NPs in dense ensembles and complex environments is crucial for the optimization of their biosensing performance. Therefore the main goal of this project is to create a comprehensive, self-consistent numerical model of such interactions including optical and photothermal effects, as well as fluid flow and biomolecule diffusion.

1.2 Outline

Detection of biomolecules by plasmonic nanoparticles is enabled by a pronounced spectral shifts of LSPR caused by the changes of the local refractive index induced by binding of an analyte molecule to a receptor molecule stabilized on nanoparticle's surface. The sensitivity is highly dependent on the size, shape and local environment of a nanoparticle.

Recent advances in the field show that single-molecule binding events can be resolved by monitoring individual nanoparticle over time. However, reliable measurement of the concentration requires to gather enough statics (binding events), which can be realized by exploiting single-nanoparticle spectroscopy within a nanoparticle ensemble, as each nanoparticle can potentially serve as an independent sensor with single-molecule resolution [2]. This approach requires ultrasensitive, background-free optical method to detect the nanoparticles in a wide field of view.

Achieving this requires extensive optimization of both the nanoparticle geometry and the detection setup. The computational model created in this project will allow to study optical phenomena at the nanoscale thus providing essential optimization tool and theoretical background for the analysis of experimental results.

The versatile model will be used to analyze recently emerging sensing techniques like the optically driven plasmonic nanomotors.

1.3 Work plan

This project will be realized in close cooperation with an experimental project being realized at the Laboratory of Applied Biophotonics aimed to build biosensing setup. The project will include three specific aims:

Aim 1. Create a comprehensive numerical model of a plasmonic nanoparticle in biological environment consisting of self-consistent solver of partial differential equations accounting for optical interactions of light beams (including vector beams) with plasmonic nanoparticles in closely spaced configurations, the photothermal effects and the diffusion of analyte molecules in the nanoparticle surrounding.

Aim 2. Use the model to identify the optimum shapes and sizes of nanoparticles for various optical detection schemas, including: (i) refractometric sensing with single gold nanorods; (ii) exploitation of field enhancement in plasmonic nanocavities; and (iii) optically-driven plasmonic nano-motors.

Aim 3. Perform biosening experiments to verify and validate the numerical model. This includes fabrication of samples and measurements using established protocols and equipment build in parallel projects.

1.4 Literature

[1] A. B. Taylor and P. Zijlstra, ACS Sensors **2**, 1103 (2017).

[2] M. A. Beuwer, M. W. J. Prins, and P. Zijlstra, Nano Lett. **15**, 3507 (2015).

1.5 Required initial knowledge and skills of the PhD candidate

The successful candidate should have good understanding of optics and nano-photonics, in particular plasmonic resonance, and experience in numerical modeling of optical phenomena.

1.6 Expected development of the PhD candidate's knowledge and skills

The PhD candidate will acquire extensive theoretical knowledge in nano-photonics, programming skills (e.g. Python) and familiarity with a commercial multiphysics simulation software (e.g. COMSOL).