The main purpose of my visit to Prof. Maier's group was to provide theoretical support in situ to some of the ongoing projects, as well as getting an overview of their experimental arrangements and techniques.

Within the projects we proposed to tackle were the following:

- Investigate the possibility of adding corrections to the polarizability prescription, including the option of dealing with materials with very large refractive indices (based on Mie theory) and the possibility of taking account of boundary effects.
- Study the possibility of including an image-dipole approach to model nanoparticles deposited on substrates (the possibility of illuminating with a Gaussian beam would be very much appreciated).
- Use our simulation capabilities to investigate the combination of plasmonic structures/antennas on metamaterial systems.

During this visit, we satisfactorily worked on two out of the three. Moreover, although the initial idea was to add FFT (Fast Fourier Transform) capabilities to the existing E-DDA code (an Extension of the Discrete Dipole Approximation), we mainly used COMSOL Multiphysics, as the applicant had never use it before, and it was widely employed within the Experimental Solid State Physics Group.

The first project we focused on was the study of dielectric solar cells. Plasmonic nanostructures have been recently investigated as a possible way to improve absorption of light in solar cells. The basic principles for the functioning of plasmonic solar cells include scattering and absorption of light due to the deposition of metal nanoparticles. Silicon does not absorb light very well. For this reason, more light needs to be scattered across the surface in order to increase the absorption. It has been found that metal nanoparticles help to scatter the incoming light across the surface of the silicon substrate. However, one important disadvantage of using metallic nanoparticles is that they absorb much of the incoming light by themselves. To overcome this problem, we suggest using high refractive index (dielectric) nanoparticles, such as GaP, whose scattering efficiency can be almost as high as that of metallic nanoparticles, but whose absorption efficiency in the visible range is very low.

In order to tackle this problem, we had to study nanoparticles deposited on substrates, making use of dipole-based models in the first instance (including dipoles embedded in dielectric slabs and an image-dipole approach). There is still some more work to do on this, but we did establish a working planning, so these results can end up in an interesting publication.

The second project we worked on was the investigation of heating effects in plasmonic nanoparticles. Metallic nanoparticles (NPs) can efficiently release heat under optical excitation. The heat generation process involves not only absorption of incident photons, but also heat transfer from the NP to the surrounding matrix. The mechanism of heat release is very simple - the laser electric field strongly drives mobile carriers inside the NPs, and the energy gained by carriers turns into heat. Then the heat diffuses away from the NP and leads to an elevated temperature of the surrounding medium. Heat generation becomes especially strong in the case of metal NPs in the regime of plasmon resonance. Plasmon resonance is a collective motion of a large number of electrons. In the case of semiconductor NPs, the heat generation rate is much weaker since heat dissipation occurs through an interband absorption process with the creation of a single mobile electron and hole (exciton). In our case, the whole process of light absorption and subsequent heat transfer between the nanostructure and the surrounding medium has been modeled by means of finite element simulations. For easy implementation and reliability of the solution, we have chosen Comsol Multiphysics 4.3a (Comsol Inc., Burlington, MA), which provides state-of-the-art routines to solve partial differential equations (PDEs). In our simulations, we have assumed the electromagnetic losses from the electromagnetic waves in the NPs as the only heat source. We furthermore assumed that the electromagnetic cycle time is short compared to the thermal time scale (adiabatic assumption).

These results are now being written in a manuscript and will be sent for publication to a high impact journal. The support received from the European Science Foundation (ESF) within the framework of the ESF activity 'New Approaches to Biochemical Sensing with Plasmonic Nanobiophotonics (PLASMON-BIONANOSENSE)' will be acknowledged and a reprint will be forwarded to the ESF Secretariat as soon as available.

We also had several scientific discussions in connection with the field of nanophotonics, specially applied to bio-sensing, which have led to several new ideas that will be studied further in our collaboration.

In summary, this visit to Prof. Maier’s Group, apart from offering me the possibility of getting introduced to the experimental techniques being developed there, has helped to start a new collaboration regarding the use of dielectric nanoantennas for spectroscopy (SERS, SEIRA), which can provide a unique platform to obtain high-impact results.