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

Project title: Optoelectronic properties of 2D material nanoflakes

1.1 Project goals

The aim of the project is theoretical characterisation of optical and electronic properties of two-dimensional nanoflakes made of graphene, hexagonal boron nitride and a representative of transition metal dichalcogenides.

The realisation of this goal has in view the creation of tunable optoelectronic devices at the nanoscale based on basic optoelectronic building blocks: conducting materials (like suitably prepared graphene) [1], semiconducting materials (like transition metal dichalcogenides) [2,3] and insulating materials (like hexagonal boron nitride) [4]. Nowadays, these materials can be combined into van der Waals structures, making it possible to create heterojunctions with required properties tunable by design, and dynamically controllable with electronic (e.g. by applying an electric voltage) or optical (by using a laser) methods [5,6].

The aim of the project is to characterise the band structure and optical response of selected nanoflakes of two-dimensional monolayer and layered flakes, including those combining different materials, in analogy to the construction of macroscopic optoelectronic devices such as tunnel transistors, ohmic junctions, Schottky barriers or light sources [7-9].

1.2 Outline

The work will be carried out in close collaboration with research centres in Karlsruhe Institute of Technology (group of Prof. Carsten Rockstuhl, nanophotonics), in Donostia/San Sebastian (group of Prof. Andres Ayueli, electronic properties of two-dimensional materials) and National Institute of Standard and Technology, Maryland, USA (Prof. Garnett Bryant, theory of low-dimensional structures). Student internships in Karlsruhe and San Sebastian are planned.

Our collaboration with the above-mentioned centres has a long history; in particular, the present PhD project is a continuation of a project developed for more than 3 years. We have published several papers on methods for characterization of plasmonic excitations in graphene nanostructures and on the influence of atomic defects on the optical response of atom chains [10-12].

The basic working tool will be the GRANAD numerical code prepared from scratch within this collaboration. It is an implementation of the quantum description of two-dimensional nanoflakes based on the methods of solid state theory (Hamiltonian of the system in the tight-binding approximation) and quantum optics (master equation for modelling dynamics of the system) as well as standard methods for modelling the distribution of electromagnetic fields or absorption spectra.

Currently, the code allows modelling of graphene and boron nitride, and includes a simplified model of transition metal dichalcogenides. The student will implement the full model of dichalcogenides and stacking monolayers into multilayer van der Waals structures.

Moreover, the student will use the code to characterise the influence of
- geometry of the investigated structures, including the type of materials, the way they are combined, the type of edges, defects,
- "controlling" external factors, i.e. electromagnetic field of laser beam or Fermi energy modulated by external voltage
on the optoelectronic properties (such as band structure, absorption spectrum, transport properties) of the investigated structures.

1.3 Work plan

12 months: Investigation of optoelectronic properties of graphene nanoflakes: characterisation of the effects of geometry, defects and external factors on the optical response (using existing code elements).

12 months: Code extensions to include the model of transition metal dichalcogenides for the particular case of molybdenum sulfide. Characterisation of the optoelectronic properties of dichalcogenide and boron nitride monolayers.

12 months: Implementation of layer stacking in a tight binding model. Characterisation of the optoelectronic properties of selected multilayer structures in the context of applications.

12 months: Additional problems and thesis preparation.

1.4 Literature

[1] Q. Bao & K. Ping Loh, *Graphene photonics, plasmonics, and broadband optoelectronic devices*, ACS Nano 6, 3677 (2012)
[2] B. Radisavljevic et al., *Single-layer MoS2 transistors*, Nat. Nano. 6, 47 (2011)
[3] J. S. Ross et al., *Electrically tunable excitonic light-emitting diodes based on monolayer WSe_2 p–n junctions*, Nat. Nano. 9, 268 (2014)
[4] B. Gil et al., *Boron nitride for excitonics, nano photonics, and quantum technologies* Nanophotonics 9, 3483 (2020)
[5] F. Xia et al., *Two-dimensional material nanophotonics*, Nat. Phot.8,899 (2014)
[6] K. Novoselov et al., *2D materials and van der Waals heterostructures*, Science 353, 6298 (2016)
[7] L. Britnell et al., *Field-effect tunneling transistor based on vertical graphene heterostructures*, Science 335, 947 (2012)
[8] L. Britnell et al., *Strong Light-Matter Interactions in Heterostructures of Atomically Thin Films*, Science 340, 1311 (2013)
[9] F. Withers et al., Nat. Mat. *Light-emitting diodes by band-structure engineering in van der Waals heterostructures*14, 301 (2015)
[10] MM Müller, M Kosik, M Pelc, GW Bryant, A Ayuela, C Rockstuhl, K Słowik *Energy-based plasmonicity index to characterize optical resonances in nanostructures*, he Journal of Physical Chemistry C 124 (44), 24331-24343 (2020)
[11] MM Müller, M Kosik, M Pelc, GW Bryant, A Ayuela, C Rockstuhl, K Słowik *From single-particle-like to interaction-mediated plasmonic resonances in graphene nanoantennas*, Journal of Applied Physics 129 (9), 093103 (2020)
[12] MM Müller, M Kosik, M Pelc, GW Bryant, A Ayuela, C Rockstuhl, K Słowik *Modification of the optical properties of molecular chains upon coupling to adatoms*, Physical Review B 104 (23), 235414 (2021)

1.5 Required initial knowledge and skills of the PhD candidate

Required: Basic quantum mechanics
Basic programming
Welcome: Basic atomic physics, light-matter interaction theory

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

The project combines various aspects of modern science and technology. The candidate

will acquire and refine knowledge in
- quantum solid state theory,
- quantum optics,
- nanophotonics and optoelectronics.

The candidate will acquire and refine the following skills:
- Python programming and modelling,
- investigating properties of materials using tight binding model, band structure modelling,
- modelling the dynamics of quantum open systems,
- modelling of optical response of photonic nanostructures,
- individual and group work, cooperation at the international level,
- presentation of scientific results in the form of papers and conference contributions.