**Brno University of Technology**
**Central European Institute of Technology BUT**

# Supervisor's report

Academic year: **2023/2024**

Student: **Mgr. Jorge Andres Navarro Giraldo**

Doctoral programme: **Advanced materials and nanosciences**

Field of study**: Advanced nanotechnolgies and microtechnogies**

Supervisor: **doc. Dr. Ing. Petr Neugebauer, Ph.D.**

Co-Supervisor: **Vinicius T. Santana, Ph.D.**

Name of doctoral thesis topic: **Theoretical Study of Low-Energy Excitations in Reduced-Dimensional Materials**

**Overall evaluation of the doctoral thesis and study period of the doctoral student:**

The PhD research of Jorge Navarro was dedicated to the study of low-energy excitations in reduced-dimensionality materials, particularly, graphene and graphite, employing several theoretical methods and focusing on the description and prediction of magneto-optical experiments at sub-THz and far infrared frequencies. The thesis investigates three different problems that arise in graphene and graphite, namely, i) the formation of spin-density waves in graphite due to the crossover from 3D to 1D electronic behavior at high magnetic fields, ii) the weak localization in graphene arising from the enhanced coherent electronic transport in a 2D system and its detection by sub-THz magneto-spectroscopy, and iii) the interplay between graphene and single-molecule magnets. The work is divided into seven chapters in addition to the introduction and appendices. The structure of the thesis is as follows. The introduction describes the importance of reduced-dimensional materials for basic research and technological applications, emphasizing the discussion on graphene and graphite, and the experimental methods available for their electrical characterization. In Chapter 1, the theoretical aspects and state of the art are introduced, explaining the effects of a magnetic field and electromagnetic radiation on the electronic properties of materials. Chapter 2 deals with a theoretical study of spin-density waves (SDW) in graphite, which appear at high magnetic fields ($\sim$ 75 T) and low temperatures. An analytic solution to the SDW energetic bands is obtained, as well as numerical solutions under some approximations that permit to find the SDW energy gap. Then, the magneto-optical spectra of the SDWs are computed, and finding the spectroscopic signatures might allow the identification of SDWs in a far-infrared spectroscopy experiment. Chapter 3 presents a study of the weak localization in graphene measured by sub-THz spectroscopy. It shows a thorough characterization of graphene samples by transport experiments and magneto-optical spectroscopy at low frequencies ($\sim$ 10 GHz) and sub-THz frequencies, and compares it with the current theoretical results of weak localization in graphene. It is demonstrated that when the frequency of the electromagnetic excitation is comparable with the characteristic scattering rate of dephasing, the spectra acquire a frequency dependence not observed before. In Chapter 4, the properties of graphene

as a substrate for the deposition of single-molecule magnets are explored. By employing density functional theory (DFT) and complete active space self-consistent field (CASSCF) theory, properties of the molecular interaction with graphene are predicted, such as binding energies, changes in the molecular geometry and electronic structure, charge transfer, and molecular magnetic properties. These predictions are compared with experimental results of high-frequency electron paramagnetic resonance and electric transport, finding good agreement between them. Chapter 5 covers the main conclusions, the references are found in Chapter 6, and Chapter 7 shows the publications and scientific outputs of the doctoral studies. Finally, the appendices cover more detailed experimental results. The thesis has 182 pages in total.

The PhD thesis is well structured and, overall, well written with minor comments/mistypes. Mr. Navarro demonstrates a high degree of competence when dealing with three related but nonetheless independent problems, which require the application of a wide range of complex theoretical and experimental methods, including quantum field theory, numerical solutions based on custom-made code, density functional theory, Raman spectroscopy, magnetotransport experiments at low temperatures, sub-THz magnetospectroscopy, among others. In the first year of his PhD studies, Mr. Navarro was awarded the prestigious Brno PhD Talent 2019 scholarship. During his studies, he attended several conferences and summer schools, including the International Conference on Magnetic Materials in Manchester, UK (ICMM2021), and the European Conference on Molecular Magnetism in Rennes, France (ECMM2022). Mr. Navarro attended two research stays in other scientific groups with a focus on the theoretical description of graphene and graphite, namely, at the National Graphene Institute in Manchester, UK (group of Prof. Vladimir Fal'ko), and at Laboratoire de Physique et Modélisation des Milieux Condensés in Grenoble, France (group of Dr. Denis Basko). He also served as a mentor in the Master's thesis of Mgr. Jan Dubský at the Brno University of Technology. He participated in numerous events for science popularisation (European researchers' nights), and was an active member of the CEITEC Student Committee, which organizes the yearly CEITEC PhD and Postdoc Retreat. During his Ph.D. studies, Mr. Navarro considerably improved his skills in experimental and theoretical science, communication, and the English language. Furthermore, he has proven to plan and execute experiments of high complexity, analyze the obtained results, and present them not only to knowledgeable professionals but to a broader audience as well. Moreover, Mr. Navarro is capable of writing scientific publications with minimal guidance. Some of his ideas had not been implemented, but they can be a good starting point for future Master's and PhD students of our group.

In our opinion, the reviewed thesis **fulfils** all requirements posed on theses aimed at obtaining PhD degree. This thesis **is** ready to be defended orally, in front of the respective committee.

Brno, date: 02/09/2024

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**doc. Dr. Ing. Petr Neugebauer, Ph.D.**

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**Vinicius T. Santana, Ph.D.**