PHD PROJECT DESCRIPTION

(4000 characters max., including the aims and work plan to de published online)

Project title: Optoelectronic Properties of Nanoflakes of Emerging 2D Materials

1.1. Project goals

The goal of the project is to apply a computational framework developed within our group for modelling the electronic, optical, and optoelectronic properties of finite nanoflakes made of emerging two-dimensional materials, with particular emphasis on borophene, phosphorene, and silicene. These materials exhibit reduced symmetry, structural anisotropy, nontrivial lattice geometries, and strong sensitivity to external control parameters, which makes them promising platforms for nanoscale photonics and optoelectronics.

The project will extend the GRANAD code developed by our team, originally designed for simulations of graphene-based nanostructures, toward new classes of 2D materials beyond standard honeycomb lattices. The main scientific objective is to identify how material composition, finite size, shape, edge termination, defects, strain, or electrostatic gating affect the optical response of atomically thin nanoflakes. Particular attention will be paid to anisotropic absorption spectra, symmetry-dependent selection rules, and nonlinear optical effects such as harmonic generation.

The project will combine tight-binding electronic-structure modelling with density-matrix-based time-dependent simulations. This approach will allow the doctoral candidate to study realistically sized nanostructures with microscopic detail while including optical driving, dissipation, and external tuning mechanisms.

1.2. Outline

The project will start with familiarisation with the theory of electronic and optical response in low-dimensional materials and with the GRANAD computational code. The next stage will involve implementation of material-specific tight-binding Hamiltonians for borophene, phosphorene, and silicene nanoflakes, including lattice geometries, onsite energies, hopping parameters, spin-orbit effects where relevant, and more complex unit cells.

The central part of the project will focus on modelling the linear optical response of finite nanostructures and identifying the influence of size, shape, anisotropy, edge type, defects, or external gating. The final scientific stage will extend the simulations toward nonlinear and dynamically controlled optoelectronic response, including selected scenarios of harmonic generation and symmetry-dependent optical transitions. The project will conclude with integration of results, preparation of publications, public release of the developed code extensions, and completion of the doctoral dissertation.

1.3. Work plan

Phase I: Theoretical and computational preparation (M1–M6)

The doctoral candidate will become familiar with the physics of emerging two-dimensional materials, including borophene, phosphorene, and silicene, and with the tight-binding description of finite nanostructures. This phase will also include training in density-matrix methods for light-driven electron dynamics and practical work with the GRANAD code.

Expected outcomes: literature review; internal methodological report; first test simulations using existing graphene, hBN, or TMDC modules.

Phase II: Implementation of material-specific tight-binding models (M4–M12)

The candidate will implement selected lattice geometries and effective Hamiltonians for borophene, phosphorene, or silicene nanoflakes. This will include material-specific hopping parameters, onsite energies, additional orbitals or spin-orbit terms where necessary, and flexible generation of finite flakes with different shapes and edge terminations. The implementation will be benchmarked against literature data, DFT results, and available analytical or numerical models.

Expected outcomes: extended GRANAD material catalogue for selected emerging 2D materials; benchmark calculations of electronic spectra and density of states; draft of the methods + electronic structure sections of the dissertation.

Phase III: Tunable linear optical response of finite nanoflakes (M11–M28)

This phase will focus on the calculation of absorption spectra, polarizability, and anisotropic optical response of finite borophene, phosphorene, or silicene nanoflakes. The candidate will investigate how the response depends on material type, flake size, shape, edge termination, defects, strain, or electrostatic gating. Particular emphasis will be placed on identifying spectral signatures of finite-size effects, edge states, and reduced symmetry. If time allows, the project can be extended by additional materials.

Expected outcomes: systematic dataset of optical spectra; identification of geometry- and material-dependent optical resonances; first peer-reviewed publication; draft of the dissertation chapter on linear optical response.

Phase IV: Tunable nonlinear optoelectronic response (M25–M42)

The candidate will extend the analysis toward time-dependent and nonlinear optical phenomena. Using the density-matrix formalism, the candidate will investigate selected scenarios of optically driven electron dynamics, anisotropic response under polarized illumination, and nonlinear effects such as second- and third-harmonic generation. The role of inversion-symmetry breaking, edge-induced symmetry reduction, defects, strain, or gating in enabling or enhancing nonlinear optical response will be analysed.

Expected outcomes: characterisation of nonlinear and externally controlled optical response; second and third peer-reviewed publications; GRANAD code extensions for selected nonlinear-response simulations.

Phase V: Integration, dissemination, and dissertation writing (M37–M48)

The final phase will be devoted to integrating the results into a coherent doctoral thesis, preparing final publications, documenting the developed computational tools, and releasing selected code extensions and simulation examples in line with open-science principles.

Expected outcomes: public release of selected GRANAD extensions with documentation and example notebooks; completed dissertation; at least three manuscripts submitted or published.

1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

[1] Dams, D., Kosik, M., Müller, M. M., Ghosh, A., Babaze, A., Szczuczko, J., Bryant, G. W., et al. GRANAD "Simulating GRAphene Nanoflakes with ADatoms", Computer Physics Communications 317, 109818 (2025) - Introduction of the GRANAD computational framework forming the methodological foundation of the proposed doctoral project.

[2] Pelc, M., Dams, D., Ghosh, A., Kosik, M., Müller, M. M., Bryant, G. W., Rockstuhl, C., et al. "Single-particle approach to many-body relaxation dynamics", Physical Review A 109, 022237 (2024) -Density-matrix and relaxation framework relevant for modelling dissipative optical dynamics in finite nanostructures.

[3] Kosik, M., Müller, M. M., Słowik, K., Bryant, G. W., Ayuela, A., Rockstuhl, C., Pelc, M. "Revising quantum optical phenomena in adatoms coupled to graphene nanoantennas", Nanophotonics 11(14), 3281–3298 (2022) - Introduction to the tight-binding approach and quantum-optical modelling of graphene-based nanostructures and light–matter interactions.

[4] Müller, M. M., Kosik, M., Pelc, M., Bryant, G. W., Ayuela, A., Rockstuhl, C., Słowik, K. "Modification of the optical properties of molecular chains upon coupling to adatoms", Physical Review B 104(23), 235414 (2021) - Illustrates the impact of atomic defects on modification of

optical response of nanostructures.

[5] Mannix, A. J., et al. "Synthesis of borophenes: Anisotropic, two-dimensional boron polymorphs", Science 350, 1513–1516 (2015). - Experimental demonstration of borophene as an emerging anisotropic 2D material.

[6] Xia, F., Wang, H., Jia, Y. "Rediscovering black phosphorus as an anisotropic layered material for optoelectronics and electronics", Nature Communications 5, 4458 (2014). - Work establishing phosphorene as a highly anisotropic platform for optoelectronics.

[7] Liu, C.-C., Jiang, H., Yao, Y. "Low-energy effective Hamiltonian involving spin-orbit coupling in silicene and two-dimensional germanium and tin", Physical Review B 84, 195430 (2011). - Theoretical basis for modelling silicene and related buckled 2D materials.

1.5. Required initial knowledge and skills of the PhD candidate

The candidate should hold a Master's degree in physics, materials science, nanotechnology, or a closely related discipline. A solid background in at least one of the following areas is required: quantum mechanics, quantum optics, solid-state physics, or computational physics.

Basic skills in numerical simulations and programming, preferably in Python, are required. Familiarity with linear algebra and basic mathematical concepts of quantum mechanics are essential. Prior exposure to tight-binding models, density-matrix formalism, electronic-structure calculations, or electromagnetic simulations will be considered an advantage.

Good command of written and spoken English, motivation, and readiness to work in an international research environment are expected.

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

The PhD candidate will develop advanced expertise in theoretical and computational science at the interface of quantum optics and solid-state physics. The candidate will learn how to construct and validate tight-binding models for finite nanostructures, simulate time-dependent electron dynamics under optical driving, and analyse linear and nonlinear optical response.

The candidate will also acquire advanced skills in modelling disorder, defects, anisotropy, finite-size effects, dissipation, and electrostatic control in nanoscale systems. By working with the GRANAD platform, the candidate will gain practical experience in extending an existing research codebase, benchmarking new implementations against literature data and complementary simulation methods, and translating physical models into efficient computational tools.

A particularly important aspect of the candidate's training will be the development of skills related to open, reproducible, and transparent computational science. The project will provide hands-on experience in scientific programming, code development, version control, validation, documentation, preparation of reusable simulation workflows, and public release of research software. The candidate will learn good practices in maintaining scientific code, preparing user-friendly examples and documentation, organizing datasets, and ensuring that numerical results can be independently reproduced and verified. These competences are increasingly essential in modern computational physics and will significantly strengthen the candidate's future research profile.

The project will be carried out within a well-established network of long-standing international collaborations with excellent research institutions abroad, including leading groups specializing in nanophotonics, atomistic modelling, quantum optics, and low-dimensional materials. These partnerships are supported by a proven record of joint research, staff exchange, research visits, and mobility of students and early-career researchers. Through interaction with these partner groups, participation in conferences, preparation of peer-reviewed publications, and possible research visits, the candidate will strengthen scientific communication skills and develop the ability to work effectively in an interdisciplinary and international research environment.

In the second half of the PhD project, the candidate will be encouraged to prepare their own grant applications, for example within NCU internal funding schemes or the NCN PRELUDIUM programme. The project will also foster independent project planning, critical analysis of numerical results, responsible research conduct, and scientific writing, culminating in the preparation of a doctoral dissertation, several research publications, and openly available computational tools useful for the broader scientific community.