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

Project title: Quantum-Nano-Optics in 2D-Material-Inspired Photonic Architectures

1.1 Project goals

The goal of the project is to develop and validate a computational framework for modeling light dynamics in 2D-material-inspired photonic lattice architectures, based on the tight-binding approach combined with density-matrix formalism. The project aims to investigate localization, disorder and defect engineering, and the role of loss and gain in structured photonic systems, identifying regimes where these effects can be harnessed for controlled light propagation and communication functionalities. An additional objective is the extension of the GRANAD code developed in our group, initially dedicated to model electronic dynamics in 2D materials, to include a dedicated photonic module enabling reproducible and scalable simulations of such architectures.

1.2 Outline

The project is structured into five phases. It begins with familiarisation with the theoretical framework and computational tools, followed by the adaptation of the tight-binding and density-matrix formalism within GRANAD to photonic lattice architectures. The core of the project focuses on disorder and defect engineering and on dynamical modeling including loss and gain mechanisms. The final phase is devoted to integration of results, dissemination, public release of the developed tools, and completion of the doctoral dissertation.

1.3 Work plan

Phase I: Familiarising with the tools (M1-M4)

Getting familiar with 1) the relation between the Schroedinger equation and dynamics of light in photonic architectures in the paraxial approximation; 2) the tight-binding model for electron dynamics in 2D materials and for light dynamics in photonic architectures; 3) the computational framework within the GRANAD environment developed in the group.

Phase II: Adaptation of the tight-binding framework in GRANAD to photonic lattice architectures (M4-M12)

Implementation and validation of photonic onsite and hopping parameters in terms of effective refractive index and mode coupling. Adaptation of density-matrix formalism to photonic propagation in lattices. Reproducing benchmark results for selected 1D and 2D lattices (e.g., SSH chain, honeycomb flake). Cross-validation of selected cases with full-wave simulations (e.g., COMSOL). Development of visualisation tools for time-resolved field propagation.

Expected outcomes: Validated photonic TB framework. Functional photonic master-equation GRANAD module. Internal methodological report. Foundation of chapter draft for the PhD thesis (methods section outline).

Phase III: Disorder and defect engineering (M9-M24)

Investigation of localisation mechanisms in 2D-material-inspired photonic lattices. Systematic study of structural disorder and its impact on band structure and density of states. Investigation of edge states and domain-wall-guided modes. Identification of regimes where disorder enhances confinement or guiding. Characterising the role of selected types of disorder, defects, and domain walls as resources rather than limitations, with applications for directional propagation, mediation of interactions between defect sites, communication.

Expected outcomes: Two peer-reviewed publications. Dataset and reproducible simulation scripts. Draft of thesis chapter on band-structure engineering and localization.

Phase IV: Dynamical modeling and loss/gain mechanisms (M20-M32)

Extention of the framework to incorporate dissipation, loss, and gain mechanisms specific to bosonic photonic systems. Implementation of relaxation operators accounting for field attenuation and amplification. Validation of dynamical results against full-wave simulations (e.g. COMSOL). Characterisation of impact of loss or gain on selected disorder-induced effects.

Expected outcomes: Functional photonic master-equation GRANAD module with extensions accounting for loss and gain. Charactersing the impact of loss or gain on selected applications in communication and guiding, identified in Phase III. 3rd peer-reviewed publication. Methodological section for thesis.

Phase V: Integration, Dissemination, and Dissertation Writing (M28-36)

Consolidation of scientific results into a coherent doctoral thesis. Finalization of publications and public release of photonic module of GRANAD with its documentation.

1.4 Literature

[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 present project. The photonic module developed in this PhD will extend this platform.

[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) - Development of the density-matrix formalism and relaxation modeling central to the dynamical and loss/gain extensions planned in this project.

[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) - Demonstrates the application of tight-binding and quantum-optical methods to structured nanophotonic systems, bridging condensed-matter and photonic perspectives.

[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 defect- and coupling-induced modification of optical response, conceptually related to defect and disorder engineering in photonic lattices.

[5] Christodoulides, D. N., *et al.* "Discrete self-focusing in photonic lattices", *Nature* 424, 817–823 (2003) - Seminal work establishing the analogy between discrete photonic waveguide arrays and tight-binding/Schrödinger-type dynamics, forming the conceptual bridge used in this project.

[6] Tran, T. T., *et al.* "Quantum emission from defect centers in hexagonal boron nitride", *Nature Nanotechnology* 11, 37–41 (2016) -Representative experimental work on defect-related optical phenomena in 2D materials, providing physical context and motivation for defect engineering in photonic analogues.

1.5 Required initial knowledge and skills of the PhD candidate

The candidate should hold a Master's degree in physics or a closely related field. A solid background in at least one of the following areas is required: quantum optics, solid-state physics, classical electrodynamics, or photonics. Basic understanding of the Schrödinger equation, band structure concepts, and light–matter interaction is expected.

Experience in numerical simulations and programming (preferably in Python) is required. Familiarity with linear algebra, differential equations, and computational methods for physics is essential. Prior exposure to tight-binding models, density-matrix formalism, or electromagnetic simulations (e.g., COMSOL or similar tools) will be considered an advantage.

Good command of written and spoken English and the ability to work both independently and within an international research team are expected.

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

During the project, the PhD candidate will develop advanced expertise in theoretical and computational photonics, with particular emphasis on tight-binding modelling and density-matrix approaches to light dynamics in structured systems. The candidate will gain experience in extending and maintaining a scientific codebase (GRANAD), including implementation of new physical models, validation, documentation, and reproducible research practices.

The candidate is expected to strengthen skills in numerical optimization, modeling of disorder and dissipative effects, and cross-validation with full-wave electromagnetic simulations. Through collaboration with international partners, conference participation, and joint publications, the candidate will develop scientific communication skills and the ability to work in an interdisciplinary research environment.

The project will also foster independent problem-solving, project planning, and scientific writing competencies, culminating in the preparation of peer-reviewed publications and a doctoral dissertation.

The project is carried out in close international collaboration, in particular with the Karlsruhe Institute of Technology (Germany) and Centro de Fisica de Materiales (San Sebastian, Spain), and the candidate will actively interact with partner groups abroad. Through joint research activities, research visits, conference participation, and co-authored publications, the candidate will acquire the skills necessary for effective work in an international scientific environment.