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

Project title: Quantum Dot Stacks as a Platform for Analog Simulation of Many-Body Hamiltonians

1.1. Project goals

The main goal of the project is to establish semiconductor quantum dot (QD) stacks, in particular, different types of nanowire quantum dots, as a controllable solid-state platform for analog simulation of selected many-body Hamiltonians.

The project will focus on identifying realistic nanostructures in which the low-energy electronic or excitonic states can be mapped onto effective lattice Hamiltonians such as: Heisenberg-type spin models (via exchange-coupled states), Su–Schrieffer–Heeger (SSH) chains (via engineered tunnel coupling modulation), and/or simplified Hubbard-like models (via competition of tunneling and Coulomb interactions).

The specific objectives are:

1. To develop a quantitative mapping between atomistic electronic structure (tight-binding + configuration interaction) and effective model Hamiltonians.
2. To identify design principles (geometry, composition, stacking, strain) enabling control over key parameters (tunneling t, interaction U, exchange J).
3. To propose experimentally feasible QD stack architectures that realize regimes of physical interest (e.g., dimerization, spin coupling, localization–delocalization crossover).

The outcome will be a physically grounded framework that connects realistic semiconductor nanostructures to canonical many-body models.

1.2. Outline

The project combines continuous media approximation (k.p) and atomistic modelling (TB), and many-body theory. At the microscopic level, the electronic structure of QD stacks will be computed using either non-atomistic k.p or atomistic tight-binding (TB), including strain, alloy disorder, and spin–orbit coupling. Many-body states (excitons, few-particle states) will be obtained using configuration interaction (CI).

The central idea is to project the full atomistic Hamiltonian onto a reduced basis of relevant localized states (e.g., dot-localized orbitals or Kramers pairs). This enables the extraction of effective parameters: tunneling amplitudes (t), Coulomb integrals (U, V), and exchange couplings (J). These parameters define an effective lattice Hamiltonian, whose structure can be engineered via QD stacking: SSH physics (alternating inter-dot couplings in engineered stacks), Heisenberg-like models (exchange between localized spins [electron or hole states]), and Hubbard-like regimes (competition between tunneling and interaction).

A key challenge, and opportunity, is that real QDs lack ideal symmetry and exhibit disorder. Rather than treating this as a limitation, the project will investigate the robustness of model

behavior under realistic perturbations/conditions.

1.3. Work plan

Year 1: Foundations and single/double QD systems

- Implementation and validation of k.p/TB+CI workflow for QD stacks.
- Study of single QDs and coupled QD pairs (tunnel coupling, exchange).
- Definition of projection procedure to extract effective parameters (t, J, Coulomb terms).
- First mapping to minimal two-site models.

Year 2: Short QD chains and emergence of model behavior

- Extension to few-dot stacks (3–6 dots).
- Engineering and analysis of non-uniform coupling (SSH-like dimerization).
- Identification of regimes where effective Hamiltonians reproduce expected spectra (e.g., bonding/antibonding structure, edge states).
- Sensitivity analysis: role of disorder, strain, and geometry.

Year 3: Many-body regimes and scaling

- Inclusion of multi-particle states (few-electron or excitonic systems).
- Exploration of Hubbard-like physics: interplay of tunneling and Coulomb interaction.
- Systematic extraction of effective parameters across a large dataset of structures.

Year 4: Inverse design and experimental relevance

- Targeting specific Hamiltonian regimes (e.g., strong dimerization, controlled exchange).
- Identification of experimentally realizable structures.
- Prediction of observable signatures (spectra, splittings, optical transitions).
- Final integration: from atomistic model → effective Hamiltonian → measurable quantities.

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

Recommended:

1. M. Zieliński, M. Korkusinski, and P. Hawrylak, Atomistic tight-binding theory of multi-exciton complexes in a self-assembled InAs quantum dot, Phys. Rev. B., 81, 085301 (2010)

2. M. Patera, and M. Zieliński, Antibonding ground states in crystal phase quantum dots, Phys. Rev. B 106, L041405 (2022)

Optional:

3. M. R. Zirnbauer, Particle-Hole Symmetries in Condensed Matter, (2020, arXiv:2004.07107)

4. D. P. Arovas et al., The Hubbard Model (2021 review; arXiv:2103.12097)

5. N. Batra, G. Sheet, Understanding basic concepts of topological insulators through the SSH model, (2019; arXiv:1906.08435)

6. J. K. Asbóth, L. Oroszlány, A. Pályi, A Short Course on Topological Insulators (2016; arXiv:1509.02295)

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 (or obtain one soon). A solid foundation in quantum mechanics, solid-state physics, and basic numerical methods is expected. Prior exposure to at least some of the following topics will be advantageous: quantum confined systems (e.g., quantum wells, quantum dots), basic concepts of many-body physics (e.g., Coulomb interaction), and introductory knowledge of model Hamiltonians (e.g., tight-binding, Hubbard, or Heisenberg models).

The candidate should possess programming skills sufficient for scientific computing (preferably in C/C++, Python, or a similar language), including the ability to work with numerical data and modify existing codes.

Familiarity with Linux/Unix environments and basic tools for data analysis and visualization will be beneficial. Previous experience with high-performance computing is not required, but will be considered an asset.

Strong analytical thinking, motivation for independent research, and the ability to work both independently and collaboratively are essential.

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

During the PhD, the candidate will develop advanced expertise at the intersection of computational condensed-matter physics and many-body theory**.**

In particular, the candidate will:

- acquire in-depth knowledge of atomistic modeling methods**,** including tight-binding approaches for semiconductor nanostructures,
- gain practical experience with many-body techniques**,** especially configuration interaction,
- learn how to derive and interpret effective Hamiltonians from microscopic models,
- develop the ability to connect realistic nanostructures with abstract theoretical models (e.g., Heisenberg, SSH, Hubbard-type systems).

The candidate will also significantly strengthen their computational skills, including:

- development and optimization of scientific code,
- work in high-performance computing environments,
- handling and analysis of large-scale numerical datasets.

In addition, the PhD training will foster:

- the ability to formulate and solve open research problems,
- scientific writing and presentation skills,
- experience in disseminating results through publications and conference presentations.

By the end of the project, the candidate will be well prepared for a research career in condensed matter physics, nanoscience, or related interdisciplinary fields combining physics and advanced computation.