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

Project title: Atom-by-atom control of spectra and topological properties of nanostructures.

1.1. Project goals

The project goals aim at understanding of spectral and topological properties of various nanostructures. We plan to utilize several atomistic many-body approaches, augmented with machine learning and global optimization techniques. We aim to understand how the details of nanostructures are related to their morphology on the atomic level. Our research will include studying the role of underlying lattice symmetry and disorder effects due to alloying or defects. We will explore both spectral and topological properties of bilayer materials formed by either two overlapping quasi-two-dimensional layers (bilayer graphene and TMDCs) or two flat, strongly coupled quantum dots embedded in the semiconductor nanowire.

1.2. Outline

Crystal phase quantum dots [AKOPIAN] are a new type of nanostructures that can be grown with monolayer precision and have atomistically sharp interfaces [ASSALI,HARMAND]. Since recently, it is also possible to develop and measure photoluminescence spectra of nanowire-embedded double quantum dots [KHOSH]. At the same time, single quantum dots are often called 'artificial atoms,' while coupled quantum dots are known as solid-state analogs of molecular systems. A new class of atomically thin coupled quantum dots has been proposed to appear in twisted transition metal dichalcogenides (TMDs) [TWIST1, TWIST2]. A twist between layers in combination with strain effects in the moiré superlattice creates an effective modulating potential well allowing particles to localize. A particularly promising is potential control of coupling between the dots by applying a perpendicular electric field [TWIST1]. The signatures of localized excitons in the moiré superlattice has already been seen [TWIST 3].

Regarding potential applications of nanowire quantum dots, the bright exciton recombination is considered as a tool for the generation of entangled photons through the biexciton-exciton cascade [JONS]. In contrast, the dark exciton recently gained significant attention as a candidate for long-lived, though optically addressable quantum bit [SCHWARTZ, ZIEL1]. Double or multiple quantum dots in nanowires, and quantum dot in twisted bilayer crystals are far less studied, and quantum dot molecules should have several advantages over single quantum dot systems e.g. in various entanglement generation schemes [KOSH].

One of the project goals is to develop theory and run highly demanding atomistic calculations for a family of nanowire-embedded artificial molecules and coupled quantum dots in twisted atomic bilayers. We aim to understand how nanostructures shapes and dimensions, and couplings between pair of nanostructures, affect their electronic and optical spectra.
To achieve this goal, we aim for several significant theoretical and computational developments. In particular, we aim to utilize machine learning techniques to solve the inverse computational problem of matching spectra to nanostructure's morphological properties. Machine learning should be of tremendous help in determining properties, such as dimensions or composition profiles

corresponding to demanded spectral properties. In a traditional approach, one is forced to study many nanostructures in function of height, diameter, shape, etc.
The multidimensional search over numerous nanostructures is, however, often impractical due to immense computational complexity. A machine learning approach should help to solve this inverse problem in a far more efficient way. The results and the knowledge gained during this process would further be significant not only from the fundamental science point of view but will also act as a guideline for experimentalists.
The project will be conducted in strong collaboration with NCN OPUS project "Artificial molecules in nanowires: atomistic calculations of excitonic spectra and machine learning", which is focused mainly on InP systems.

1.3. Work plan

1. Development of tight-binding theoretical models aiming for the description of a broad family of nanostructures.
2. Implementation of theoretical models as computer programs.
3. Codes parallelization and initial large-scale calculations.
4. Combining new codes with existing tools for machine learning and global optimization.
5. Nanostructural calculations and analysis of results.
6. Writing scientific papers and PhD thesis; auxiliary calculations

1.4. Literature

[AKOPIAN] Nano Lett. 10, 1198 (2010)
[ASSALI] Nano Letters 17, 6062 (2017)
[CIRLIN] J. Phys. D Appl. Phys. 50, 484003 (2017)
[HARMAND] Phys. Rev. Lett. 121, 166101 (2018)
[JONS] Scientific Reports 7, 1700 (2017)
[KHOSH] Nature Communications 8, 15716, (2017)
[MBB1] Nano Lett. 12, 6 6206 (2012)
[MBB2] Nano Lett. 2016, 16, 1081 (2016)
[ROZANSKI] Phys Rev B 94, 045440 (2016)
[SCHWARTZ] Phys. Rev. X 5, 011009 (2015)
[ZIEL1] Phys Rev B 91, 085403 (2015)
[ZIEL2] Phys. Rev. B 81, 085301 (2010)
[TWIST1] Phys Rev B 102, 075413 (2020)
[TWIST2] Sci. Adv.3, e1701696 (2017)
[TWIST3] Phys. Rev. Lett. 126, 047401 (2021)

1.5. Required initial knowledge and skills of the PhD candidate

- commitment and good motivation for work in science!
- a degree in physics or similar
- ability to read scientific papers in English
- good computer programming skill

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

- practical skills and expert knowledge in the field of nanostructure theory
- experience in high-performance computation
- practical understanding of machine learning algorithms and software
- ability to write scientific papers in English
- ability to present results of own research in a professional manner
- teamwork skills