DOCTORAL PROJECT PROPOSAL
DOCTORAL SCHOOL OF EXACT AND NATURAL SCIENCES AST
NICOLAUS COPERNICUS UNIVERSITY IN TORUŃ
Contest 007, May 2025

| | | |
|---|---|---|
| **Project discipline: Physics** | | |
| **Project title (in English)** | | |
| Designing spin models using nanographenes | | |
| **Project title (in Polish)** | | |
| Projektowanie modeli spinowych za pomocą nanografenów | | |
| **Project submitter(s)/Contact person** | | |
| dr hab. Pawel Potasz, prof. UMK<br>degree/title, first and last name | ppotasz@umk.pl, 532 599 002<br>e-mail, phone number | |
| | WFAiIS<br>organizational unit | |
| **Suggested supervisors and mentors** | | |
| 1) main supervisor* | | |
| dr hab. Pawel Potasz, prof. UMK<br>degree/title, first and last name | ppotasz@umk.pl, 532 599 002<br>e-mail, phone number | |
| | WFAiIS<br>organizational unit | |
| | field: | physics |

<table>
<tr><td colspan="3">2) co-supervisor*</td></tr>
<tr><td rowspan="3">.....<br>degree/title, first and last name</td><td colspan="2">.....<br>e-mail, phone number</td></tr>
<tr><td colspan="2">.....<br>organizational unit</td></tr>
<tr><td>field:</td><td></td></tr>
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<tr><td colspan="3">3) auxiliary supervisor*<br><br>A short justification for the need for auxiliary supervisor in this project</td></tr>
<tr><td rowspan="3">.....<br>degree/title, first and last name</td><td colspan="2">.....<br>e-mail, phone number</td></tr>
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*According to the Regulations of the Doctoral School of Nicolaus Copernicus University in Toruń (Resolution No. 30 of 23.04.2024), the scientific supervision of the preparation of the doctoral dissertation is provided **by the supervisor or supervisors OR the supervisor and the auxiliary supervisor**.
Meaning, you can provide the data of **a maximum of 2 people**: **2 co-supervisors OR the main supervisor and auxiliary supervisor.**

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

**Project title:** Designing spin models using nanographenes

### 1.1. Project goals

The project goals aim at designing spin models from open-shell nanographenes in order to create realistic quantum simulators [1]. Open-shell nanographenes characterize by nonzero magnetic moments, or no net magnetic moment but antiferromagnetic coupling [2]. Using advanced quantum mechanical tools, we will determine conditions for realization of spin models from nanographenes that include one dimensional chains with half-integer and integer spins, finite size spin systems and two-dimensional crystals.

### 1.2. Outline

Exact analytical solutions have been developed for relatively simply microscopic quantum models supported by powerful field theoretic and computational approaches, providing greater insight into the emergence of these complex phases and their physical properties. Understanding of spectral and topological properties of various quantum mechanical correlated models is challenging due exponential growth of Hilbert space with a system size, while experimental investigation of such systems might answer to crucial questions regarding fundamental laws governing the quantum world. This approach belongs to a general class of quantum simulations [1]: designing quantum mechanical systems that mimic the other ones that cannot be solved neither numerically using standard (classical) computers, nor using analytical methods. On-surface synthesize has led to the discovery of open-shell nanographene as promising building blocks for creating quantum spin models [2]. Recent fabrication of synthetic spin 1 chain with characteristic edge states of Haldane symmetry-protected topological phase [3] open a bottom-up approach to study strongly correlated topological phases in purely organic materials. Synthesized carbon nanostructures of various shapes allow one to create systems with magnetic order and controllable magnetic exchange coupling. Realization of isotropic spin ½ chain designed in nanographenes and observation of spinons show huge potential in these quantum simulators [4-6]. We plan to utilize several atomistic many-body approaches to investigate electronic properties of nanographenes and to map their low spectrum to effective spin models.

## 1.3. Work plan

We will start from already implemented tight-binding, Hartree-Fock and exact diagonalization methods to derive accurate fermionic model of various nanographenes. This will allow us to investigate the basic properties of the systems. Next, we will determine parameters of effective spin models by direct comparison of low energy spectra. We will realize different spin models from nanographenes that include one dimensional chains with half-integer and integer spins, finite size spin systems and two-dimensional crystals. Next, we will relate our findings to the experiments. Demonstration the Haldane gap and topological edge states [3] of one-dimensional spin-1 chains made of pi-electron magnetic nanographene highlighted the potential of combined on-surface synthesis and STM atomic detection. Scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) are used to characterize and manipulate spin degrees of freedom. Spin excitations can be probed using inelastic electron tunneling spectroscopy (IETS). In the conventional theory for IETS, the zero bias conductance is related to the square of the local magnetization of the ground state through resonant tunneling via the Kondo effect. We will model the dI/dV spectroscopy following Ref. [7]. Electron scattering that can produce a spin flip can be related to electrons that tunnel from tip to sample, exciting from the ground state in the process, and scattering between the substrate electrons. We will confront our simulations of STM spectra with the latest experiments.

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


[1] R. Feynman, Int. J. Theor. Phys. 21, 467 (1982).
[2] D. G. de Oteyza and T. Frederiksen, J. Phys.: Cond. Mat. 34, 443001 (2022).
[3] S. Mishra et al. Nature 598, 287–292 (2021).
[4] Z. Yuan et al. arXiv:2408.08612 (2024).
[5] X. Su et al. arXiv:2408.08801 (2024).
[6] C. Zhao et al. arXiv:2408.10045v1 (2024).
[7] J. Fernández-Rossier, Phys. Rev. Lett. 102, 256802 (2009).


## 1.5. Required initial knowledge and skills of the PhD candidate

- MSc in physics.
- Fundamental knowledge about quantum physics.
- Basic experience in many-body quantum mechanical calculations
- Basic experience in lattice models will be an advantage
- Skills in computer programming (C, Matlab, Python or Fortran)

- Communication skills and ability for working in a team
- English in speaking and writing (advanced)

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

- practical skills and expert knowledge in the field of nanostructure theory and spin models
- practical understanding of quantum many-body effects
- experience in high-performance computation
- ability to write scientific papers in English
- ability to present results of own research in a professional manner
- teamwork skills

## 2. INFORMATION ON ACADEMIC ACHIEVEMENTS BY SUGGESTED PROJECT SUPERVISORS (REQUIRED FOR EACH PERSON INVOLVED)

| A. Suggested supervisor | dr hab. Pawel Potasz, prof. UMK<br>degree/title, first and last name |
|---|---|
| **a. Grants obtained in the last 5 years** | |
| NCN OPUS 2021 - 2025 | |
| **b. H-index value** | |
| according to Google Scholar | 19 |
| according to Scopus | 17 |
| **c. Number of quotations** | |
| according to Google Scholar | 1733 |
| according to Scopus | 1202 |
| **d. Value of Field Weighted Citation Impact in the last 5 years (by SciVal database)** | 1.63 |
| **e. List of 4 major academic papers published or accepted for publication in the last 4 years, IFs** | |
| 1) Y. Saleem, T. Steenbock, E. R. J. Alhadi, W. Pasek, G. Bester, **P. Potasz**, *Superexchange Mechanism in Coupled Triangulenes Forming Spin-1 Chains*, Nano Letters **24**(24), 7417-7423 (2024). (pkt. 200 MNiSW)<br>https://doi.org/10.1021/acs.nanolett.4c01604 | |
| 2) N. Morales-Durán, Nai Chao Hu, **P. Potasz**, A. H. MacDonald, *Nonlocal Interactions in Moiré Hubbard Systems*, Phys. Rev. Lett. **128** (21), 217202 (2022). (pkt. 200 MNiSW)<br>https://doi.org/10.1103/PhysRevLett.128.217202 | |
| 3) **P. Potasz**, M. Xie, A. H. MacDonald, *Exact diagonalization for magic-angle twisted bilayer graphene*, Phys. Rev. Lett. **127**, 147203 (2021). (pkt. 200 MNiSW)<br>https://doi.org/10.1103/PhysRevLett.127.147203 | |
| 4) **P. Potasz**, N. Morales-Durán, N. C. Hu, A. H. MacDonald, *Itinerant ferromagnetism in transition metal dichalcogenide moiré superlattices*, Phys. Rev. B **109** (4), 045144 (2024). (pkt. 140 MNiSW)<br>https://doi.org/10.1103/PhysRevB.107.054411 | |
| **f. List of promoted doctoral candidates: last names, titles of doctoral dissertations, names of universities, year and field of graduation** | |
| | |
| **g. Information on currently supervised doctoral theses (list of doctoral students, name of the** | |

| doctoral school, year of education, and topic of the doctoral dissertation, please indicated those on "the fifth year"- extension) |
| --- |
| Weronika Pasek, Doctoral School of Exact and Natural Sciences, IV year, title:<br>Realization of quantum simulators in low dimensional structures for strongly correlated systems. |
| **h. Description of previous (and potential) scientific cooperation with other academic centers in the last 5 years (max. 1 page)** |
| PP has ongoing collaborations with A. H. MacDonald from University of Texas at Austin (USA), and P. Hawrylak from University of Ottawa (Canada), M. Korkusiński from National Research Council of Canada, and M. Bieniek from Wrocław University of Technology. Past collaborations include, e.g., . J. Fernandez-Rossier from International Iberian Nanotechnology Laboratory in Braga (Portugal). This collaboration might be refreshed due to related topics. These collaborations focused on understanding physics of low dimensional systems and the role of correlations. These includes topological, magnetic and electronic properties of two dimensional moire superlattices, like twisted bilayer graphene and transition metal dichalcogenide bilayers. These collaborations aimed to directly compare results of accurate theoretical models with experimental results. Altogether these collaborations resulted in many joint papers published in the last decade in such journals as Nano Letters, Physical Review Letters, and Physical Review B. |
| **i. Scientific resume of the supervisor (can be added as a separate file)** |
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**4. DECLARATION OF TECHNICAL/EXPERIMENTAL/FINANCIAL RESOURCES SUFFICIENT AND NECESSARY TO COMPLETE THE PROJECT**

I declare that I am able to provide the technical/equipmental support and financial resources necessary to carry out this doctoral project.

Paweł Potasz

07-05-2025, Toruń
place, date

signature of project submitter

I declare that ~~I HAVE/~~DO NOT HAVE financial resources for a doctoral scholarship as part of a project from external sources:.....

*project name/souces name*

Paweł Potasz

07-05-2025, Toruń
place, date

signature of project submitter

**5. DECLARATION CONCERNING THE AUTHORSHP OF PROJECT IDEA**

I declare that the author of the idea for the doctoral project is: dr hab. Pawel Potasz, prof. UMK

Paweł Potasz

07-05-2025, Toruń
place, date

signature of project submitter

**6. DECLARATION CONCERNING CONSENT TO TRANSFER OF PROJECT SUPERVISION IF NEEDED**

I declare that should the PhD candidate be accepted to the Doctoral School of Exact and Natural Sciences and started the project but for some reasons a change of the supervisor is necessary, I **AGREE/DO NOT AGREE** to transfer the substantive supervision of the project to another person designated by the Director of the Doctoral School of Exact and Natural Sciences of the Nicolaus Copernicus University in Toruń.

Paweł Potasz

07-05-2025, Toruń
place, date

signature of project submitter

**7. DECLARATION CONCERNING THE POSSIBILITY OF PUBLISHING THE CONTENT OF THE PROJECT**

I declare that the description of the project submitted to the contest from point 1 and basic scientific CV of a prospective supervisor, can be published on the website of Doctoral School of Exact and Natural Sciences, Nicolaus Copernicus University in Toruń.

Paweł Potasz

07-05-2025, Toruń
place, date

signature of project submitter