Nanophysics Center, Reykjavik University
Annual Report 2023

Members of the group

During 2023 the Nanophysics Center (nano.ru.is) had five full time faculty staff: Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Kristinn Torfason. Gunnar Þorgilsson and Muhammad Taha Sultan were still external collaborators, partly affiliated with us. Abdul Raman Mallah and Hákon Örn Árnason were postdoctoral scientist. Anna Sitek, from Wroclaw University (Poland) and Movaffaq Kateb from Chalmers University (Sweden) were also collaborators within two different projects. The group included several PhD students: Hadi Rezaie Heris, Hamed Gramizadeh, Elham Aghabalaei Fakhri (who became postdoc in April), Rachel Elizabeth Brophy, and Yuan Zhou. Two new BS students continued to work on research projects with us, Arnar Jónsson and Jasmín Lára Jóhannsdóttir. Two guest graduate students from Romania visited the group for two months (November-December) and worked with us on collaborative projects: Bianca Solomonea and Calin Pantis.

Main research projects: participants, results, work in progress

Thermoelectric transport in core-shell nanowires.
This research was performed under a Rannis project obtained by Hadi, for an extension to a forth year of his doctoral program, until May 2023. Hadi calculated the thermoelectric and heat currents associated with electrons in semiconductor nanowires with polygonal cross sections, using the Green's function method. A more extended manuscript including the effect of impurities was sent for publication at the end of the year. He also performed a new series of calculations concerning the effect of phonons on the thermoelectric currents in nanowires, known as the phonon drag effect, and he successfully defended his PhD thesis in April 2023.

Spin-orbit interaction in core-shell nanowires.
Anna Sitek made significant progress with implementing the k·p method to obtain the spin-orbit interaction in tubular nanowires of a polygonal geometry. The k·p equation is solved numerically on a polar grid using two steps. In the first step we neglected the Coulomb interaction and solved the equation for a set of finite values of the wave vectors. In the second step we included the Coulomb interaction. She got the first results in the second part of 2023, showing that the spin-orbit effect of Rashba type decreases with decreasing the shell thickness. The results were presented in a conference, followed by the publication is the proceedings, and a more extended manuscript on this subject is in progress.

Spin-orbit effect on the magnetoresistance of 2D systems.
The project ended in April 2023 when the student Hamed Gramizadeh defended his PhD thesis, titled "Magnetoresistance and spin-orbit interaction in complex 2DEG systems: a study of Shubnikov-de Haas oscillations". Two publications resulted from this thesis, see publication list.

Halide-perovskite materials for photovoltaic applications.
This is an EEA funded project in collaboration with a group from National Institute for Materials Physics, Romania, and another group from University of Oslo. The doctoral student Rachel Brophy and the former postdoctoral researcher Movaffaq Kateb (now at Chalmers) performed computational studies on the migration of iodine ions in the perovskite material $CH_3NH_3PbI_3$ (MAPI) using molecular dynamics simulations with the LAMMPS software. They showed that the iodine vacancy has a higher mobility than

the iodine interstitial ion, and that iodine vacancies can be immobilized by hydroxyl ions (OH^-) possibly generated by water molecules. In parallel Kristinn Torfason performed calculations of the electronic states and band alignment at the interface between MAPI and a layer of copper and nickel oxide, using the Siesta software based on DFT, and found that a small amount of hydroxyl ions do not significantly affect the density of states and band alignment. The result was presented in a IEEE conference and published in the proceedings. A more detailed manuscript is in preparation, to be submitted to a journal.

Breath sensors based on Silicon nanowires.
This is a new Rannis project led by Halldór Svavarsson, started in 2023. Using the piezoresistive effect of silicon nanowires (studied and published by our group in 2022), and in combination with the sensitivity to humidity, we showed that silicon nanowires can be used as a sensor of human breath, with potential application in medicine, especially in sleep studies. Elham Aghabalaei Fakhri, who successfully defended her PhD thesis in March 2023, on the piezoresistance of silicon nanowires, continued to work with us on this project, together with Hákon Örn Árnason. A journal paper was published on the breath sensing. The doctoral student Rachel Brophy also worked with silicon nanowires and tested their response to humidity in a laboratory specialized in gas sensors in Germany, at Tubingen University, where it was found that these nanowires are also sensitive to NO_2, in the presence of humidity. A paper on this effect was submitted for publication.

Electronic properties of vacuum diodes.
The doctoral student Yuan Zhou worked on utilizing machine learning to compute the effects of image charge on surface polarization in a conducting capped cylinder. This work was done in collaboration with Calin Pantis and Amanda Preda, students from the Horia Hulubei National Institute for Physics and Nuclear Engineering in Romania. Electric surface field was estimated using deep neural networks (DNN) and physics informed multiple image charge models. Preliminary results were presented at ICOPS 2023 in Santa Fe, New Mexico. The doctoral student Hákon Örn Árnasson completed his simulations of the photoemitted current due to a short laser pulse and defended his PhD the second week of 2023. Subsequently, extended the results of that research and presented them at ICOPS 2023 and in a scientific paper in the IEEE Transactions on Electron Devices. Arnar Jónsson undertook a series of simulations to investigate beam expansion from an electron source with small diameter in a high aspect ratio diode, as well as investigating the temporal and spatial evolution of emittance in a beam from a microemitter. We received a grant from the US Air Force Office of Scientific Research amounting to $140,000 to support research on parametrization of the RUMDEED code, modeling of strong-field emission, emission from core-shell nanowires and ionization. We prepared and submitted a project grant and a grant of excellence to the Icelandic Research Fund, both of which were unfortunately rejected.

Grants and other financial resources

Geometry effect on phonon drag in core-shell nanowires, The Icelandic Research fund, doctoral grant, Hadi Rezaie Heris, 6.5 mil. ISK (2021-2022).

Towards perovskite large area photovoltaics (PERLA-PV), EEA funded project, with partners from National Institute for Materials Physics, Romania, and another group from University of Oslo.

Funds from individual research accounts provided by the Department of Engineering, Reykjavik University, were used for participation at conferences, for guest scientists, and for software license.

Funds for the PhD students Elham Aghabalaei Fakhri, Hamed Gramizadeh, Yuan Zhou, and Rachel Brophy were provided by the research funds of Reykjavik University.

The postdoctoral researcher Abduk Rahman Mallah has been funded by the EEA project called SiSal-Pilot, on a novel way to produce solar-grade silicon by using by-product from aluminum smelters Acronym SiSal-Pilot.
Electron emission physics simulations, US Air Force Office of Scientific Research (AFSOR), PI Ágúst Valfells (2023-2025).

Windows on Science travel grants for Ágúst Valfells and Kristinn Torfason, US Air Force Office of Scientific Research (AFSOR).

Environmental humidity sensor based on silicon nanowires, Andrei Manolescu and Halldór Svavarsson, 1 mil ISK from Landsvirkjun obtained through the Sustainability Institute Forum of Reykjavik University.

Events related to the activity of the center (short visits, presentations, theses, etc.)

18 January, Hákon Örn Árnason defended his PhD thesis entitled "Electronic properties of microstructured surfaces: Photoemission for pulsed electron beams in a microdiode, and pressure effects on resistance in silicon nanowires" with external examiner Prof. Einar Örn Sveinbjörnsson from University of Iceland.

12 January, Gur Lubin from Weizmann Institute of Science, Israel, delivered the talk entitled Heralded Spectroscopy: A new probe for nanocrystal multiexciton photophysics.

March 2023, Rachel Brophy spent two weeks at the University of Tübingen, Germany, where she completed a course on Chemical Gas Sensors and participated at measurements regarding detection of NO_2 with arrays of silicon nanowires.

31 March, Thesis Defense Elham Aghabalaei Fakhri, Fabrication and characterization of silicon nanowires for pressure sensing applications, examiners Prof. István Csarnovics, from University of Debrecen (Hungary), and Prof. Anna Kaźmierczak-Bałata, from Silesian University of Technology, Gliwice, Poland.

3 April, Prof. Istvan Csarnovics from Material Science Centre at the University of Debrecen gave a presentation entitled "Creation and investigation of metallic nanoparticles for sensing application, SERS".

17 April, Hadi Rezaie Heris, PhD thesis defense, Charge and heat transport in semiconductor core-shell nanowires with temperature bias, examiner Dr. Mircea Trif from Institute of Physics, Polish Academy of Sciences, Warsaw.

18 April, Dr. Mircea Trif gave a presentation entitled "Quantized spin pumping in topological ferromagnetic-superconducting nanowires".

26 April, Visitors from a DEVCOM US Army Research Laboratory.

28 April, Hamed Gramizadeh, PhD thesis defense, Magnetoresistance and Spin-Orbit interaction in Complex 2DEG Systems: A Study of Shubnikov-de Haas Oscillations, examiner Dr. Martin Veis, Charles University, Prague.

18-19 May, Ágúst Valfells and Kristinn Torfason visited the Air Force Research Laboratory in Albuquerque, New Mexico to give a presentation of our work and discuss collaboration opportunities on modelling of electron emission.

25 May, Andrei Manolescu, Summary of recent work at the Nanophysics Center of Reykjavik University, presentation at Nordita Board meeting.

15 June 2023, Andrei Manolescu, Electronic properties of semiconductor tubular nanowires, presentation at the 6-th International Symposium - Nanotechnology from Academy to Industry, Holon Institute of Technology, Israel.

2-13 October, visit of Prof. Catalina Marinescu from Clemson University, South Carolina, USA.

10 -17 October, Elham visited the group of Prof. Anna Kaźmierczak-Bałata, at Silesian University of Technology, Gliwice, Poland, and performed measurements on detection of NH3 with our arrays of silicon nanowires.

1 November, visit at RU of two representatives of Air Force Office of Scientific Research (AFSOR) to discuss the status of our project "Electron emission physics simulations", funded by them.

20 October – 19 December, Bianca Solomonea and Calin Pantis, Master and PhD students at University of Bucharest, visited our group with an EEA funded project for mobility. Bianca worked with Rachel on molecular dynamics simulations and NEB calculations of MAPI, and Calin worked with Yuan on an algorithm based on machine learning to calculate the electrostatic field associated with image charges in a fiber of carbon nanotubes.

14 December, Prof. Andri M. Gretarsson from Embry-Riddle Aeronautical University, USA, gave the presentation "The Astronomical Reach of Gravitational Wave Detectors is Determined by Solid-State Physics".

Journal papers (e-prints, accepted, or published)

H. Gramizadeh, D. R. Candido, A. Manolescu, J. C. Egues, S. I. Erlingsson, Efficient method to calculate energy spectra for analyzing magneto-oscillations, accepted for publication in Phys. Rev. B (2024) arXiv:2306.02503.

D.R. Candido, S.I. Erlingsson, H. Gramizadeh, J.V.I. Costa, P.J. Weigele, D.M. Zumbühl, and J. Carlos Egues, Beating-free quantum oscillations in two-dimensional electron gases with strong spin-orbit and Zeeman interactions, Phys. Rev. Res **5**, 043297 (2023).

G. Thorgilsson and S.I. Erlingsson, Lead Green's functions from quadratic eigenvalue problems without mode velocity calculations, Phys. Rev. E **108**, 055304 (2023).

H. Ö. Árnason, K. Torfason, A. Manolescu, Á. Valfells, Simulation of short pulse photoemission in a micro-diode with implications for optimal beam brightness, accepted for publication in IEEE Transactions on Electron Devices, DOI 10.1109/TED.2024.3351096 (2024) arXiv:2301.06123.

E. A. Fakhri, M. T. Sultan, A. Manolescu, S. Ingvarsson, H. G. Svavarsson, Application of p and n-type silicon nanowires as human respiratory sensing device, Sensors 23, 9901 (2023).

V. Gudmundsson, V. Mughnetsyan, N. R. Abdullah, C.-S. Tang, V. Moldoveanu, A. Manolescu, Controlling the excitation spectrum of a quantum dot array with a photon cavity, Phys. Rev. B 108, 115306 (2023), arXiv:2305.11544.

R. E. Brophy, M. Kateb, K. Torfason, G. A. Nemnes, H. G. Svavarsson, I. Pintilie, A. Manolescu, Effect of pressure on the dynamics of iodine defects in MAPI: An atomistic simulation, J. Phys. Chem. C 127, 7938 (2023), arXiv:2302.05696.

M. Kateb and A. Manolescu, Distinct melting behavior of partially oxidized Cu nanoparticles and nanowires, submitted for publication, arXiv:2302.02219 (2023).

H. R. Heris, K.O. Klausen, A. Sitek, S. I. Erlingsson, and A. Manolescu, Effect of impurities on charge and heat transport in tubular nanowires, Nanotechnology 34, 335401 (2023), arXiv:2302.02164.

C. -A. Pantis-Simut, A. T. Preda, L. Ion, A. Manolescu, G. A. Nemnes, Mapping confinement potentials and charge densities of interacting quantum systems using conditional generative adversarial networks, Machine Learning: Science and Technology 4, 025023 (2023), arXiv:2301.02122.

K. O. Klausen, A. Sitek, S. I. Erlingsson, A. Manolescu, Electron-hole coherence in core-shell nanowires with partial proximity induced superconductivity, Phys. Rev. B 107, 035423 (2023) arXiv:2206.04830.

N. R. Abdullah, H. O. Rashid, A. Manolescu, V. Gudmundsson, Interaction effects in a two-dimensional AlSi6P nanosheet: A first-principles study on the electronic, mechanical, thermal, and optical properties, Physica B: Condensed Matter 652, 414627 (2023), arXiv:2108.00387.

N. R. Abdullah, Y. H. Azeez, B. J. Abdullah, H. O. Rashid, A. Manolescu, V. Gudmundsson, Role of planar buckling to the electronic, thermal, and optical properties of Germagraphene nanosheets, Materials Science in Semiconductor Processing 153, 107163 (2023) arXiv:2210.04247.

N. Filipoiu, Anca G. Mirea, Sarah Derbali, C. -A. Pantis-Simut, D. -V. Anghel, A. Manolescu, Ioana Pintilie, Mihaela Florea, G. A. Nemnes, Optoelectronic and stability properties of quasi-2D alkylammonium based perovskites, Physical Chemistry Chemical Physics 25, 3323 (2023), arXiv:2210.04596.

K. O. Klausen, A. Sitek, S. I. Erlingsson, A. Manolescu, Flux-periodic oscillations in proximitized core-shell nanowires, Nanotechnology 34, 345001 (2023), arXiv:2209.13076.

See also http://nano.ru.is/publications

Contributions to conferences

R. E. Brophy, M. Kateb, I. Ghitiu, N. Filipoiu, K. Torfason, H. G. Svavarsson, G. A. Nemnes, I. Pintilie, A. Manolescu, OH- ions can reduce the iodide migration in MAPI, 2023 International Semiconductor Conference (CAS), Sinaia, Romania, IEEE Xplore Digital Library https://ieeexplore.ieee.org/abstract/document/10303698 (2023).

A. Sitek, A. Manolescu, Low-energy electronic states in tubular wires, ICTON 2023 Bucharest, IEEE Xplore Digital Library https://ieeexplore.ieee.org/document/10207280 (2023).

H.Ö. Árnason, K. Torfason, A. Manolescu, A. Valfells. Space-charge effects on short-pulse photoemission. ICOPS 2024, Santa Fe, New Mexico, USA.

Y. Zhou, A. Preda, K. Torfason, A. Manolescu, A. Valfells, Machine learning approach for calculating image charge effects in non-planar cathodes. ICOPS 2024, Santa Fe, New Mexico, USA.

Research plans for 2024

Electrical characterization of respiratory sensors based on silicon nanowires.

Silicon nanowires as gas sensors: detection of NH_3 and SO_2

Molecular dynamics of perovskite materials for photovoltaics applications.

Proximity induced superconductivity in tubular semiconductor nanowires.

Spin-orbit coupling in core-shell nanowires.

Transport in nanowires exposed to mechanical stress.

Simulations combined with machine learning of emission and propagation of electrons in vacuum microdiodes.

Development of parametric models for electron emission and propagation.

Space-charge effects on strong-field emission.