Nanophysics Center, Reykjavik University
Annual Report 2018

Members of the group

The Nanophysics Center (Website nano.ru.is) had twelve members during 2018. Five members are faculty staff, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Gunnar Þorgilsson (who is at ISOR, but still partly affiliated with us). Anna Sitek and Kristinn Torfason are postdoctoral researchers. Anna moved back to Poland in September 2018, but she will return to RU in February 2019. Muhammad Taha Sultan, Miguel Urbaneja Torres, and Hákon Örn Árnason are PhD students. Hákon Valur Haraldsson is a Master student. Roberto Aceto is a BS student working on a research project with us. In addition Hifsa Shahid was hired in September 2018 on a postdoctoral position, to start in the beginning of 2019.

Main research projects: participants, results, work in progress

Magnetoresistance oscillations in systems with spin-orbit coupling.
This is a collaboration between Sigurður I. Erlingsson and Prof. J. Carlos Egues at the University of Sao Paulo, Sao Carlos. The main result is an equation that describes beatings in the Shubnikov-de Haas oscillations in a 2D electron gas with both Rashba and Dresselhaus interaction. The central feature of the project is a new approximation scheme that works well for strong spin-orbit coupling and high Landau-level index. This year a new experiment was published with magnetoresistance resistance measurements with strong spin-orbit coupling and we had to improve our approximation method to be able to describe those measurements. The updated manuscript is in preparation with input from the experimental group of Prof. Dominik Zumbuhl at the University of Basel that does magnetoresistance measurements.

Topological insulators.
We finished our work on magnetic impurities in helical edge states in topological insulators. The results have been published in 2018, see publication list. This project involved Dr. Karel Vyborny from Institute of Physics in Prague and Simon Wozny (student) and Dr. Wolfgang Belzig from the University of Konstanz. We also investigated electronic transport in topological insulator nanowires in the presence of impurities, both potential and magnetic ones. This work has been published, see publication list. This is project involving Dr. Jens H. Bardarson at KTH in Stockholm. We have already outlined extensions on this project.

Electronic transport in open nanosystems in the presence of photons.
Andrei Manolescu participated in the project on electronic transport through open systems coupled to cavity photons led by Vidar Guðmundsson from University of Iceland. The funding was obtained by VG from the Icelandic Research Fund in 2016. The results obtained in 2018 are on the thermoelectric transport in such systems, with the main collaborator Nzar Abdullah, former PhD student of the group. Also, two new directions were initiated: transport through two quantum dots coupled by photons, with Valeriu Moldoveanu, and transport in the presence of phonons instead of photons, with Margherita Zuppardo.

Optical properties of core-shell semiconductor nanowires.
Anna Sitek, Miguel Urbaneja, Kristinn Torfason and Andrei Manolescu worked together on the many-body states of valence and conduction electrons in core-shell nanowires with polygonal cross section, and obtained exciton spectra with Coulomb interaction included. The work began in 2017 and was published

in 2018 in Nano Letters. The Coulomb interaction was included both in a configuration interaction approach and in an electron-hole model. The electron-hole model was used by Anna Sitek to interpret experimental results obtained by the group of Hubert Krenner from Augsburg on the optical emission produced by surface acoustic waves along hexagonal GaAs nanowires.

Electronic transport in core-shell semiconductor nanowires.
Miguel Urbaneja continued his PhD project with conduction steps expected in core-shell nanowires with hexagonal, square, and triangular cross section. A paper on this subject, with the contribution of several other members of the group, was published in Phys. Rev. B. The paper also includes the nonlinear I-V characteristics and the expected anisotropy of it when a magnetic field perpendicular to the nanowire is rotated. The results are expected to be confirmed by the experimental group in Jülich, Germany. Miguel also performed a series of calculations of the radiated field by a prismatic core-shell nanowire under an AC current presented at the ICTON (IEEE) conference and another series on the absorption of light by such a nanowire using COMSOL Multiphysics software.

Silicon nanowires.
Hákon Örn Árnason finalized his Master project and made a new series of arrays of Silicon nanowires. Preliminary experiments performed by Dr. Rodica Plugaru, collaborator from Romania, showed very promising piezoresistance effects of the nanowires embedded in a pressurized gas. A Rannis project proposal was submitted in June to continue this research at RU.

Au nanocups
Halldor G. Svavarsson has been working on sensors application of a plasmonic device based on periodic arrays of gold-nanocups. In collaboration with Magnussons' group at UTA, USA. Halldór was a co-applicant of an EEA project proposal on plasmon-enhanced optical sensing of pollutants – submitted 01 October. In collaboration with Romanian partners and Innovation Center in Iceland

TiO_2 thin films with embedded GeSi nanoparticles.
This project started in 2016 and it is funded by Rannis with an M-ERA.NET collaboration with National Institute of Materials Physics from Romania. The PhD student Muhammad Taha Sultan, under the close supervision of Halldór Svavarsson, grew high quality TiO_2 layers with GeSi nanoparticles using Hi Power Impulse Magnetron Sputtering. Taha wrote two papers on the optical characteristics of annealed and hydrogenated samples, one published in Applied Surface Science and the other one under review.

Electronic properties of vacuum diodes.
Kristinn Torfason continued to improve the capabilities of the molecular dynamics code, adding the following features: calculate the emittance, velocity distribution, Shockley–Ramo current, inclusion of resistors in series with the diode, the case with two emitters for planar field emission, and cylindrical diodes. The possibility to study surface inhomogeneities was added to the code and is being studied. Steps to optimize the code for running on a GPU have started. Emission from graphene is now possible using the code. The MS student Hákon Valur Haraldsson performed calculations of the charge distribution and space-charge shielding between neighboring field emitters and a manuscript is in preparation for a journal publication. The PhD student Hákon Örn Árnason prepared GaAs cathodes emitters to be tested in 2019 for photoemission and field emission.

Comparison of different numerical methods for self-energy calculations.
Gunnar Þorgilsson and Sigurður I. Erlingsson are working on a project where different methods for calculating self-energies are compared. The self-energy is central quantity that is required to calculate transport in the scattering formalism. There is no clear consensus in the literature about which method is the fastest numerically. The goal of this project is to compare the different methods and the standard physics based methods to the more mathematical problem of solving quadratic matrix equations.

Grants and other financial resources

High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications (PhotoNanoP) M-ERA.NET project 2016-2019, in collaboration collaboration with National Institute of Materials Physics from Romania. RU team leader Halldór Svavarsson, RU budget 108000 Euro.

Core-shell nanoantennas, The Icelandic Research Fund, PI Andrei Manolescu, 41.3 mil. ISK (2016-2019).

DC vacuum-microdiode arrays as tunable THz sources, The Icelandic Research Fund, PI Ágúst Valfells, 44.9 mil. ISK (2017-2020)

Vacuum electronics, The Icelandic Research Fund, postdoctoral fellowship Kristinn Torfason, 24.5 mil ISK (2017-2020)

Molecular dynamics simulations for emission and propagation of electrons in cathode nanostructures, US Air Force Office of Scientific Research (AFSOR), PI Ágúst Valfells, 180000 USD (2018-2021).

Funds for the Nanophysics Center provided by the School of Science and Engineering were used for the acquisition of a vacuum pump.

Funds from individual research accounts provided by the School of Science and Engineering were used for travel to conferences, for guest scientists, for software license, and for the acquisition of a vacuum chamber.

Funds for three PhD positions were obtained from Reykjavik University within a new research fund established in 2018.

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

16 January, Hákon Valur Haraldsson has the presentation on his final graduation project entitled “Field emission in micro vacuum devices”

6-21 January, visit of Dr. Valeriu Moldoveanu from INFM Romania, collaborator on time dependent electronic transport at nanoscale

7 – 13 February, visit of Patrick Zellekens, PhD student at Research Center, Juelich, Germany, collaborator on electrical transport in core-shell nanowires.

14 February, Anna Sitek has a presentation entitled “Corner and side states in prismatic semiconductor shells” at 5th International Workshop on the Optical Properties of Nanostructures, OPON2018, Münster

6 April, Master thesis defense by Birgir Hrafn Hallgrímsson, “Fabrication of periodic silicon nanowires for possible thermoelectric and solar cell applications”

25 April, Ágúst Valfells gives talk entitled “Molecular dynamics simulations of vacuum diodes” at the 19th International Vacuum Electronics Conference, Monterey CA.

1 June, Master thesis defense by Hákon Örn Árnason, “Silicon Nanowires - Photovoltaic and Thermoelectric applications”

11-14 June, visit of Prof. Mauro Paternostro from Queen’s University Belfast, and introductory talk on quantum thermodynamics.

18-19 June, visit of Dr. Nathaniel Lockwood from AFOSR, US, to discuss the new project on molecular dynamics simulations of vacuum diodes.

5 July, Miguel Urbaneja Torres has an invited talk entitled “Radiated fields by polygonal core-shell nanowires” at ICTON 2018 in Bucharest

18 July, Andrei Manolescu, invited talk “Localization of electrons in semiconductor based core-shell nanowires”, Singapore University of Technology and Design.

9 August, Kristinn Torfason, talk “Modelling Nano- and Microscale Vacuum Electronics. A molecular dynamics approach” at NEMO 2018 IEEE conference in Reykjavik.

24 August, Halldór Guðfinnur Svavarsson has his inaugural talk as a full Professor at RU.

13-20 September, Dr. Nicolina Pop and Dr. Felix Iacob from University of Timisoara, Romania, visited our group to prepare an application for a common project on plasma physics at nanoscale to EEA funding.

10 October, Muhammad Taha Sultan, oral presentation “Enhanced photoconductivity of SiGe-trilayer stack by retrenching annealing conditions” at CAS 2018, Sinaia, Romania

11 October, Halldór G. Svavarsson gave a talk via Skype, on a meeting with our Romanian collaborators, summarizing the work of RU at the closure of the M-ERA-NET project PhotonanoP.

10-24 November, the second visit of Dr. Valeriu Moldoveanu from INFM Romania, collaborator on time dependent electronic transport at nanoscale

2-7 December, visit of Dr. Jens Barðarson, our Icelandic collaborator from KTH Stockholm.

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

G. A. Namnes, T. L. Mitran, A. Manolescu, D. Dragoman, Electric and thermoelectric properties of graphene bilayers with extrinsic impurities under applied electric field, submitted for publication, arXiv:1812.08672 (2018).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Thermoelectric inversion in a resonant quantum dot-cavity system in the steady-state regime, submitted for publication, arXiv:1812.05665 (2018).

G. A. Nemnes, T. L. Mitran, A. Manolescu, Gap prediction in hybrid graphene - hexagonal boron nitride nanoflakes using artificial neural networks, submitted for publication, arXiv:1812.04394 (2018).

G. A. Nemnes, C. Besleaga, A. G. Tomulescu, L. N. Leonat, V. Stancu, A. Manolescu, I. Pintilie, The hysteresis-free behavior of perovskite solar cells from the perspective of the measurement conditions, submitted for publication**,** arXiv:1812.03855 (2018).

M. T. Sultan, A. Manolescu, J. T. Gudmundsson, K. Torfason, G. A. Nemnes, I. Stavarache, C. Logofatu, V. S. Teodorescu, M. L. Ciurea, H. G. Svavarsson, Enhanced photoconductivity of SiGe nanocrystals in SiO2 driven by mild annealing, Applied Surface Science, **469**, 870 (2019) https://doi.org/10.1016/j.apsusc.2018.11.06

V. Gudmundsson, H. Gestsson, N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Moldoveanu, Coexisting spin and Rabi-oscillations at intermediate time in electron transport through a photon cavity, submitted for publication, arXiv:1809.06930 (2018).

G. A. Nemnes, T. L. Mitran, A. Manolescu, D. Dragoman, Electric field effect in boron and nitrogen doped graphene bilayers, Computational Materials Science **155**, 175 (2018).

M. Urbaneja Torres, A. Sitek, S. I. Erlingsson, G. Thorgilsson, V. Gudmundsson, A. Manolescu, Conductance features of core-shell nanowires determined by the internal geometry, Phys. Rev. B **98**, 085419 (2018) arXiv:1805.10929.

T. D. Stanescu, A. Sitek, A. Manolescu, Robust topological phase in proximitized core-shell nanowires coupled to multiple superconductors, Beilstein Journal of Nanotechnology **9**, 1512 (2018) arXiv:1804.05446.

A. Sitek, M. Urbaneja Torres, K. Torfason, V. Gudmundsson, A. Bertoni, A. Manolescu, Excitons in core-shell nanowires with polygonal cross sections, Nano Lett. **18**, 2581 (2018)

S. Wozny, K. Vyborny, W. Belzig, S.I. Erlingsson, Gap formation in helical edge states with magnetic impurities, Phys. Rev. B **98**, 165423 (2018)

S. I. Erlingsson, J. H. Bardarson, A. Manolescu, Thermoelectric current in topological insulator nanowires with impurities, Beilstein Journal of Nanotechnology **9**, 1156 (2018), arXiv:1803.04507 .

G. A. Nemnes, Cristina Besleaga, A. G. Tomulescu, Alexandra Palici, L. Pintilie, A. Manolescu, Ioana Pintilie, How measurement protocols influence the dynamic J-V characteristics of perovskite solar cells: theory and experiment, Solar Energy **173**, 976 (2018), arXiv:1803.00285 .

N. R. Abdullah, T. Arnold, C.-S. Tang, A. Manolescu, V. Gudmundsson, Photon-induced tunability of the thermospin current in a Rashba ring, J. Phys.: Condens. Matter **30**, 145303 (2018), arXiv:1712.03386**.**

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Effects of photon field on heat transport through a quantum wire attached to leads, Phys. Lett. A **384**, 199 (2018), arXiv:1711.01210.

N. R. Abdullah, C. S. Tang, A. Manolescu, V. Gudmundsson, Spin-dependent heat and thermoelectric currents in a Rashba ring coupled to a photon cavity, Physica E **95**, 102 (2018), arXiv:1707.08416 .

V. Gudmundsson, N. R. Abdullah, A. Sitek, H. S. Goan, C. S. Tang, A. Manolescu, Current correlations for the transport of interacting electrons through parallel quantum dots in a photon cavity, Phys. Lett. A **382**, 1672 (2018), arXiv:1707.08295 .

V. Gudmundsson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.-S. Tang, A. Manolescu, Electroluminescence caused by the transport of interacting electrons through parallel quantum dots in a photon cavity, Annalen der Physik 530, 1700334 (2018), arXiv:1706.03483 .

H. G Svavarsson, J. E. Valberg, H. Arnardottir, A. Brynjolfsdottir, Carbon dioxide from geothermal gas converted to biomass by cultivating coccoid cyanobacteria, Environmental technology 39, 2097-2104 (2018)

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

Contributions to conferences

M. T. Sultan, J. T. Gudmundsson, A. Manolescu, M. L. Ciurea, H. G. Svavarsson, The Effect of H2/Ar Plasma Treatment Over Photoconductivity of Sige Nanoparticles Sandwiched Between Silicon Oxide Matrix, CAS 2018 Sinaia, IEEE Xplore Digital Library https://ieeexplore.ieee.org/abstract/document/8539761 pp 257-260 (2018).

M.T. Sultan, J. T. Gudmundsson, A. Manolescu, M. L. Ciurea, C. Palade, A. V. Maraloiu, H. G. Svavarsson, Enhanced Photoconductivity of SIGE-Trilayer Stack by Retrenching Annealing Conditions, CAS 2018 Sinaia, IEEE Xplore Digital Library https://ieeexplore.ieee.org/abstract/document/8539775 pp 61-64 (2018).

C. Palade, A. Slav, O. Cojocaru, V. S. Teodorescu, S. Lazanu, T. Stoica, M. T. Sultan, H. G. Svavarsson, M. L. Ciurea, Enhanced Photocurrent in GeSi NCs / TiO2Multilayers, CAS 2018 Sinaia, IEEE Xplore Digital Library https://ieeexplore.ieee.org/abstract/document/8539740 (2018)

M. Urbaneja Torres, A. Sitek, V. Gudmundsson, A. Manolescu, Radiated fields by polygonal core-shell nanowires, ICTON 2018 Bucharest, IEEE Xplore Digital Library https://ieeexplore.ieee.org/document/8473825 pp 1-4 (2018) arXiv:1804.07959 .

K. Torfason, A. Manolescu, Á. Valfells, Modelling Nano-and Microscale Vacuum Electronics A molecular dynamics approach, IEEE MTT-S International Conference on Numerical Electromagnetic and Multiphysics Modeling and Optimization (NEMO), Reykjavik, https://ieeexplore.ieee.org/abstract/document/8503192 (2018)

K. Torfason, A. Manolescu, Á. Valfells, High-fidelity Molecular Dynamics of Vacuum Nanoelectronics, 31st International Vacuum Nanoelectronics Conference (IVNC), Kyoto, https://ieeexplore.ieee.org/abstract/document/8520287 (2018)

K. Torfason, H. V. Haraldsson, Á. Valfells, A. Manolescu, IEEE International Vacuum Electronics Conference (IVEC), Monterey CA, https://ieeexplore.ieee.org/abstract/document/8391553 (2018)

K. Torfason, Á. Valfells, A. Manolescu, Molecular Dynamics Code for Simulations of Vacuum Nanodiodes, 45th IEEE International Conference on Plasma Science (ICOPS), Denver CO, (2018)

Research plans for 2019

Thermoelectric and heat conduction of nanowires. (With a new PhD student and a new postdoc.)

Piezoresistance of arrays of Silicon nanowires.

Lateral optical absorption of arrays of Silicon nanowires.

Majorana states in tubular nanowires: core shell vs. topological insulators. (With a new PhD student.)

Electromagnetic absorption and plasmons in core-shell nanowires (Miguel Urbaneja)

Shubnikov – de Haas oscillations and spin-orbit coupling. (With new PhD student.)

Topological insulators: Transport in multi-terminal topological insulator and superconductor heterostructures.

Vacuum electronics: Preparation of cathodes and measurements (With new postdoc.). Use the molecular dynamics code to study surface inhomogeneities. Add thermionic emission to the code and study its effects with surface inhomogeneities. Possibly include circuit elements in the analysis. Finish optimizing the code for running on GPU. Experiment on 2 dimensional Child-Langmuir law.