# Nanophysics Center, Reykjavik University
# Annual Report 2016

## Members of the group

The Nanophysics Center (Website nano.ru.is) grew from six to eleven members during 2016. Five members are faculty staff, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Gunnar Þorgilsson. Two members are postdoctoral researchers, Kristinn Torfason, and Anna Sitek, Anna moving to our group in August, for one year. At the end of the summer (August-September) two PhD students arrived and started their 3-years program, Muhammad Taha Sultan and Miguel Urbaneja Torres, and also one Master's student started his one-year project, Hákon Örn Árnason. In November the BS student Hákon Valur Haraldsson joined the group within a project on electron dynamics in nanodiodes.

## Main research projects: participants, work in progress, results

*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. The manuscript is in preparation and they are interacting with the experimental group of Prof. Dominik Zumbuhl at the University of Basel that does magnetoresistance measurements..

*Topological insulators.*
Sigurður Erlingsson has continued his work on magnetic impurities in topological insulators. The analytical work done by an undergraduate student last year served as a motivation to do numerical modeling on the effects of magnetic impurities. The goal of this project is to compare the results of the diagrammatic method with the numerics, and determine whether transport measurements (the conductance) will yield more information about the effects of the magnetic impurities than optical methods (the density of states). This project involves Dr. Karel Vyborny from Institute of Physics in Prague and Simon Wozny from the University of Konstanz.

*Electronic transport in open nanosystems in the presence of photons.*
This work is on electronic states and transport in nanosystems coupled to cavity photons, described with the generalized non-Markovian master equation, with the participation of Andrei Manolescu, in collaboration with Viðar Guðmundsson and his group from University of Iceland, including Anna Sitek. The funding was obtained by the collaborator from the research funds of the University of Iceland. The main achievement in 2016 was the steady-state solution of the density matrix of the electron-phonon system, with several hundreds of states, obtained by vectorization of the master equation in the Liouville space. With this method both fast and slow electron-phonon dynamics could be obtained.

*Optical properties of core-shell semiconductor nanorings.*
This was the main activity of Anna Sitek, who moved from a postdoctoral position at University of Iceland in the group of Viðar Guðmundsson, to the Nanophysics Center, at 1 August 2016. Together with Andrei Manolescu she calculated many-body states of electrons with Coulomb interaction in polygonal core-shell nanorings. One remarkable results is that singlet two-electrons states can be situated in the gap

between corner and side states, if the later is sufficiently large as it happens for triangular or square polygons. This effect opens the possibility to measure by optical experiments the strength of the Coulomb interaction in such samples. This result was accepted for publication in Scientific Reports in the last days of 2016.

*Electronic transport in core-shell semiconductor nanowires.*
Andrei Manolescu, together with Sigurður Erlingsson and Anna Sitek, and other external collaborators, performed calculations of the conductance oscillations in hollow cylindrical nanowires in transversal magnetic field, in order to observe the role of the snaking states. The results showed Aharonov-Bohm oscillations corresponding to closed orbits of electrons surrounding the longitudinal contour of the nanowire. This result was experimentally confirmed by the group of Thomas Schäpers from Forschungszentrum Jülich and was published in a two papers, one theoretical and one experimental. Another property related to the snaking states is the change of sign of thermoelectric currents, obtained numerically by Sigurður Erlingsson and Andrei Manolescu (manuscript in preparation.) Andrei Manolescu spent most the first semester in a sabbatical leave, at Clemson and West Virginia Universities in USA and at University of Balearic Islands in Mallorca, Spain, working on transport in core-shell nanowires.

*Thermo and photovoltaic application of Silicon nanowires.*
The project is done in cooperation with the Nanophotonic Device group at University of Texas at Arlington (UTA). Halldór Svavarsson together with Master's student Hákon Örn Árnason made a new setup and started measurements of thermal conductivity of arrays of Silicon nanowires. Until the end of the year the measurements were in the calibration stage. By now, Hákon has also prepared flat p-n junctions by diffusion of antimony into silicon wafer for photovoltaic applications. The funding of this project is provided by the Energy Fund of the National Power Company of Iceland (Landsvirkjun).

*$TiO_2$ 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. A manuscript on Photoconductivity of GeSi nanoparticles embedded in $TiO_2$ matrix is now in preparation.

*Molecular dynamics simulations of vacuum diodes.*
Kristinn Torfason performed calculations of field emission from a metallic tip, with his own computer code, in collaboration with Ágúst Valfells and Andrei Manolescu. The electron propagation to the anode is described with the method of molecular dynamics. The main challenge was to include the image charge of the electrons in the proximity of the cathode, which was done using a local spherical approximation. The results were published in Physics of Plasmas. The BS student Hákon Valur Haraldsson joined the team and started a series of calculations of charge bunching in cylindrical vacuum diodes which are very promising for a possible publication next year. Ágúst Valfells also wrote a review paper on the physics of vacuum diodes in collaboration with Peng Zhang, Lay Kee Ang, Y.Y. Lau and John Luginsland. This paper was accepted for publication in Applied Physics Reviews. Ágúst Valfells spent the fall term of 2016 on sabbatical leave at the University of Michigan where he primarily worked on modelling of electron emission into diodes, and on Rutherford scattering in the cathode region as a source of emittance.

*I-V characteristics of solar cells based on halide-perovskite materials.*
This project (acronym Perphect) is an international cooperation with the National Institute of Materials Physics from Bucharest, University of Oslo, and University of Iceland, funded by an EEA research grant. The Nanophysics Center organized the annual project meeting on 3-4 November 2016. The main results in 2016 were on the dynamic I-V characteristics of perovskite based solar cells, where a hysteresis

phenomenon is present due to the slow electric polarization associated with the migration of negative Iodine ions. The contributors to this project in 2016, on the RU side, were Kristinn Torfason, Halldór Svavarsson, and Andrei Manolescu. Kristinn Torfason performed numerical simulations using his own code with molecular dynamics.

*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. A manuscript is being prepared.

**Grants and other financial resources**

Perovskites for photovoltaic efficient conversion technology, The Romanian/EEA Research Programme, Project EEA-JRP-RO-NO-2013-1-0116, PI Ioana Pintilie (National Institute of Materials Science, Romania), RU team leader Andrei Manolescu, total funds 1.25 mil. EUR, RU budget 82589 Euro, 2014-2017, funded by EEA.

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).

Use of silicon nanowires for electricity production from solar light, Landvirkjun project grant. PI Halldór Svavarsson, 3 mil ISK (2016-2017)

Funds from individual research accounts provided by the School of Science an Engineering were used for travel to conferences and for guest scientists.

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

11 February, visit from Dr. David Abergel, assistant professor at NORDITA and talk entitled “2D materials and their heterostructures”

2 May. Halldór Svavarsson gave a presentation, PhotoVoltaics-Solar Energy Converted to Electricity, on seminar on Materials for Sustainable Energy Conversion in Reykjavik University

2 May, visit of Prof. Heiner Linke from University of Lund, Sweden, and talk entitled “Nanoscience for cleaner, smarter energy”, within the same seminar on Materials for Sustainable Energy Conversion organized at RU.

19 May, visit of Prof. Dr. Carlos Sa De Melo professor at Georgia Tech, and talk entitled “Who is the Lord of the Rings in the Zeeman-spin-orbit Saga: Majorana, Dirac or Lifshitz?”

22-24 May. Halldór Svavarsson visited our collaborators at the National Institute of Materials Physics in Romania. He gave a talk there entitled Large arrays of ultra-high aspect ratio periodic silicon nanowires obtained via top–down route, http://www.infim.ro/seminars/general-seminar-dr-halldor-gudfinnur-svavarsson

1 June, Andrei Manolescu, talk entitled "Geometry dependent electronic states in core-shell nanowires", University of Balearic Islands, Palma de Mallorca, Spain.

22 June, Andrei Manolescu, talk entitled "Time dependent quantum transport treated with the generalized master equation", Queen´s University Belfast, UK.

28 July – 7 August, visit of Dr. George Alexandru Nemnes from University of Bucharest, related to the Perphect project.

19 August, *How did this happen? –a random walk through science*. Research activity overview by Ágúst Valfells related to his promotion as a full professor.

23 September, presentation by A. Valfells entitled Molecular Dynamics for Simulation of Vacuum Nanoelectronics, Nuclear Engineering Seminar, Department of Nuclear Engineering Purdue University.

25-29 September, visit of Prof. Andrea Bertoni, from University of Modena, Italy, and talk entitled Electron and hole gases in core-shell nanowires (26 Sept.)

3 November, Annual meeting of EEA funded project Perphect, on solar cells based on halide-perovskite materials, with the participation of international collaborators: Ioana Pintilie (PI), Cristina Besleaga Stan and Neculai Plugaru from National Institute of Materials Physics, Romania, Bengt Gunnar Svensson form University of Oslo, and Sveinn Ólafsson and Eiran Örn Sveinbjörnsson from University of Iceland.

2 – 19 November Dr. Neculai Plugaru, from National Institute for Materials Science, Bucharest, related to the Perphect project.

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

P. Zhang, A. Valfells, L. K. Ang, J. W. Luginsland, and Y. Y. Lau, 100 years of the physics of diodes, Applied Physics Reviews (2017, accepted in November 2016).

G. A. Nemnes, C. Besleaga, A. G. Tomulescu, I. Pintilie, L. Pintilie, K. Torfason, A. Manolescu, Dynamic electrical behavior of halide perovskite based solar cells, Solar Energy Materials & Solar Cells 159, 197 (2017, accepted in September 2016), arXiv:1606.00335.

A. Sitek, M. Tolea, M. Nita, L. Serra, V. Gudmundsson, A. Manolescu, In-gap corner states in core-shell polygonal quantum rings, Scientific Reports **7**, 40197 (2017, accepted in December 2016).

V. Gudmundsson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.–S. Tang, A. Manolescu, Time-dependent current into and through multilevel parallel quantum dots in a photon cavity, submitted to publication, arXiv:1611.09453 (2016).

T. H. Jonsson, A. Manolescu, H.-S. Goan, N. R. Abdullah, A. Sitek, C.-S. Tang, V. Gudmundsson, Efficient determination of the Markovian time-evolution towards a steady-state of a complex open quantum system, submitted to publication, arXiv:1610.03223 (2016).

K. Torfason, A. Valfells, A. Manolescu, Molecular dynamics simulations of field emission from a prolate spheroidal tip, Physics of Plasmas **23**, 123119 (2016), arXiv:1608.06789.

C. Besleaga, L. E. Abramiuc, V. Stancu, A. G. Tomulescu, M. Sima, L. Trinca, N. Plugaru, L. Pintilie, G. A. Nemnes, M. Iliescu, H. G. Svavarsson, A. Manolescu and I. Pintilie, Iodine Migration and Degradation of Perovskite Solar Cells Enhanced by Metallic Electrodes, J. Phys. Chem. Lett. 7, 5168 (2016).

S. Heedt, A. Manolescu, G. A. Nemnes, W. Prost, J. Schubert, D. Grützmacher, T. Schaepers, Adiabatic Edge Channel Transport in a Nanowire Quantum Point Contact Register, Nano Lett. **16**, 4569 (2016).

A. Manolescu, G. A. Nemnes, A. Sitek, T. O. Rosdahl, S. I. Erlingsson, V. Gudmundsson, Conductance oscillations of core-shell nanowires in transversal magnetic fields, Phys. Rev. B 93, 205445 (2016), arXiv:1601.01477.

V. Gudmundsson, T. H. Jonsson, A. L. Bernodusson, N. R. Abdullah, A. Sitek, H.-S. Goan, C.-S. Tang, A. Manolescu, Regimes of radiative and nonradiative transitions in transport through an electronic system in a photon cavity reaching a steady state, Annalen der Pysik, DOI 10.1002/andp.201600177, arXiv:1605.08248 (2016).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Optical switching of electron transport in a waveguide-QED system, Physica E 84, 280 (2016), arXiv:1602.04979.

V. Gudmundsson, A. Sitek, N. R. Abdullah, C.-S. Tang, A. Manolescu, Cavity-photon contribution to the effective interaction of electrons in parallel quantum dots, Annalen der Physik 528, 394 (2016) arXiv:1505.03181.

J. Capps, D. C. Marinescu, A. Manolescu, Spin Seebeck effect in an (In,Ga)As quantum well with equal Rashba and Dresselhaus spin-orbit couplings, Phys. Rev. B 93, 085307 (2016).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Cavity-photon controlled thermoelectric transport through a quantum wire, ACS Photonics 3, 249 (2016), arXiv:1507.06574.

R. Chirla, A. Manolescu, C. P. Moca, Transmission of a microwave cavity coupled to localized Shiba states, Phys. Rev. B 93, 155110 (2016), arXiv:1512.08093.

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Competition of static magnetic and dynamic photon forces in electronic transport through a quantum dot, J. Phys. Cond. Matt. 28, 375301 (2016) arXiv:1512.00392.

A. Sitek, G. Thorgilsson, V. Gudmundsson, A. Manolescu, Multi-domain electromagnetic absorption of triangular quantum rings, Nanotechnology 27, 225202 (2016), arXiv:1511.05596 .

G. A. Nemnes, A. Palici, A. Manolescu, Transparent boundary conditions for time-dependent electron transport in the R-matrix method with applications to nanostructured interfaces, Computer Physics Communications 208, 109 (2016), arXiv:1506.02993.

Joanna M Zajac and Sigurdur I Erlingsson, Temperature dependency of resonance fluorescence from InAs/GaAs quantum dots: Dephasing mechanisms, Phys. Rev. B **94**, 035432 (2016).

Halldor Gudfinnur Svavarsson, Birgir Hrafn Hallgrimsson, Manoj Niraula, Kyu Jin Lee and Robert Magnusson, Large arrays of ultra-high aspect ratio periodic silicon nanowires obtained via top–down route, Applied Physics A **122**, 1 (2016).

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

**Contributions to conferences**

A. Sitek, G. Thorgilsson, V. Gudmundsson, A. Manolescu, Electronic states in core-shell quantum rings, ICTON 2016 Trento, IEEE Xplore Digital Library http://ieeexplore.ieee.org/document/7550580/ (2016).

R Magnusson, J W Yoon, M Niraula, K J Lee and H G Svavarsson, Resonance-based nanophotonic device technology: Filters, reflectors, and absorbers, In *2016 IEEE Aerospace Conference*. (March 2016), 1-13.

G. A. Nemnes, C. Visan, D. V. Anghel, A. Manolescu, Molecular dynamics of halogenated graphene - hexagonal boron nitride nanoribbons, IC-MSQUARE Conference 2016, J. Phys: Conf. Series 738, 012027 (2016), arXiv:1606.00725.

G. A. Nemnes, C. Besleaga, A. G. Tomulescu, I. Pintilie, L. Pintilie, K. Torfason, A. Manolescu, Dynamic electrical behavior of halide perovskite based solar cells, E-MRS 2016, Warsaw, Poland, 19-22 September 2016 http://www.european-mrs.com/meetings/2016-fall

G. A. Nemnes, Adela Nicolaev, T. L. Mitran, N. Plugaru, A. Manolescu, S. Antohe, Band alignment in perovskite solar cells with $Cu_2O$ as hole transporter material, E-MRS 2016, Warsaw, Poland, 19-22 September 2016 http://www.european-mrs.com/meetings/2016-fall

A. Sitek, G. Thorgilsson, V. Gudmundsson, and A. Manolescu, Controllable properties of polygonal quantum rings, 4th International Workshop on the Optical Properties of Nanostructures (OPON), Wrocław, Poland, 17–19 February 2016, http://www.opon2016.pwr.edu.pl/

A. Sitek, G. Thorgilsson, V. Gudmundsson, and A. Manolescu, Few electrons in core-doubleshell rings, The International Conference on Semiconductor Mid-IR Materials and Optics (SMMO) Lisbon, Portugal, 21-24. March 2016, http://www.smmo.org/2016/index.php

G. A. Nemnes, Adela Nicolaev, T. L. Mitran, N. Plugaru, A. Manolescu, S. Antohe, Band alignment in perovskite solar cells with $Cu_2O$ as hole transporter material, Energy Materials and Nanotechnology, Cancun. Mexic 5-9 June 2016, http://www.emnsummer.org/

V. Stancu, A. G. Tomulescu, M. Sima, C. Besleaga, L. Stoflea, L. Pintilie, I. Pintilie, A. Nemnes and **A.** Manolescu, Aging effects in hybrid perovskite solar cells, 5th International Conference from Nanoparticles and Nanomaterials to Nanodevices and Nanosystems (IC4N), 2016, Porto Heli, Greece, June 26-30, http://www.uta.edu/ic4n/

H.G. Svavarsson, B.H. Hallgrimsson, M.N. Niraula, K.J. Lee, R. Magnusson, Periodic silicon nanowires with ultra-high aspect ratio obtained via top-down route in *3rd NANOSMAT-USA Conference*, University of Texas, Arlington, USA, 18-20 May 2016, http://www.nanosmat-usa.com/

**Research plans for 2017**

$TiO_2$ thin films with embedded GeSi particles: fabrication, optical, and electrical characterization.

Majorana states in core-shell nanowires.

Thermoelectric transport in core-shell nanowires.

Core-shell nanoantennas: current distribution on the surface of core-shell nanowires and characteristics of radiated electromagnetic field.

Vacuum electronics: Design and inception of experiment on THz generation (depending on funding). Modified Paschen curves at high pressure and gap spacing. Discrete particle effects and the role of surface inhomogeneity in microgap breakdown. Origins of emittance. Multifactor discharge (depending on funding –this would be part of a MURI grant funded by the Air Force Office of Scientific Research).

Solar cells based on perovskites: Hysteresis curves obtained from molecular dynamics computer simulations.

Topological insulators: Transport in topological insulator and superconductor heterostructures. Magnetic impurities in topological insulators, transport and optical properties.

Silicon nanowires: Thermal and Photovoltaic applications of silicon nanowires. A grant application for purchasing Solar-simulator will be sent to Rannis or/and Energy Fund of the Icelandic National Power Company (Landsvirkjun)