Nanophysics Center, Reykjavik University
Annual Report 2014

Members of the group

In 2014 the Nanophysics Center (Website nano.ru.is) included the following members: Four faculty, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, and Sigurður Ingi Erlingsson; three postdoctoral researchers, Gunnar Þorgilsson, Kristinn Torfason, and Charles Goehry; two PhD students, Marjan Ilkov and Abhishek Kumar; one research assistant, Tómas Örn Rosdahl; one Master student, Birgir Hrafn Hallgrímsson.

Main research projects: participants, results, funding

1. Non-Markovian electron dynamics in nanosystems with implications on fluorescence optical spectra. The participants were Sigurður Ingi Erlingsson and Abhishek Kumar in collaboration with Bill Coish from McGill University, Montreal. This project was in the final year and ended up with the PhD thesis of Abhishek Kumar. The funds for 2014 were provided by the Canadian collaborator, and for previous years by the Icelandic Research Fund.

2. Electronic transport in nanosystems assisted by cavity photons described with the generalized non-Markovian master equation, with the participation of Andrei Manolescu, in collaboration with Viðar Guðmundsson and PhD students from University of Iceland. The project is part of an ongoing research on time dependent electron transport in nanosystems. The financial support in 2014 was obtained by the collaborator from the Icelandic Research Fund and from the research funds of the University of Iceland.

3. Topological insulators based on artificial superlattices, a project performed by Sigurður Ingi Erlingsson in cooperation with Carlos Egues from University of Sao Paulo. The purpose of the project is to obtain conductive edge states in an electronic system by engineering a periodic potential with appropriate wavelength and amplitude. A related project in collaboration with Karel Vyborny from Institute of Physics in Prague involves studying transport in the presence of magnetic impurities. This project is not properly funded, the only financial support being travel funds provided by the School of Science and Engineering of RU.

4. Transport and optical properties of core-shell nanowires made of semiconductor materials. The participants were Andrei Manolescu and Tómas Örn Rosdahl in cooperation with Thomas Schäpers from Forschungszentrum Jülich, Anna Sitek from Wroclaw University of Technology, and Viðar Guðmundsson from University of Iceland. The results obtained in 2014 describe oscillations of the conductance in the presence of magnetic fields reported in the Master thesis of Tómas Örn finalized in May 2014 at University of Iceland. Between June-December 2014 Tómas Örn worked as a research assistant in the Nanophysics Center, and in spring 2015 he will start as a PhD student in Delft. Another direction within this project was the study of the optical absorption due to the localization of electrons in a polygonal shell, performed in cooperation with Anna Sitek who became a postdoc at University of Iceland in August 2014. This is an ongoing project which started in 2012 and not yet funded from a grant. Travel and other research funds obtained from the School of Science and Engineering were very helpful in 2014.

5. Thermoelectric and heat transport in Silicon nanowires. The participants were Halldór Svavarsson and Birgir Hrafn Hallgrímsson. Another contributor was Florian Maudet, an exchange student from France, during the summer 2014. The project intends to obtain an increased thermoelectric (Seebeck) voltage in

nanowires compared to the effect in the bulk, due to the suppression of the phonon modes transverse to the nanowire and the corresponding loss on heat. The funding is provided by Landsvirkjun.

6. Plasmonic periodic arrays of metallic cavities (nanocups) for sensors applications. Participant was Halldór Svavarsson in cooperation with the Nanophotonic Device group at University of Texas at Arlington (UTA). The project aims to design a simple method to fabricate periodic nanostructure suitable for diagnostic applications. A simple and versatile method based on use of laser interference lithography and metal deposition has been developed. The method is suitable for making large area of periodic structures of metallic nanocups. Its utility in determining concentration of specific compound in solutions has been demonstrated experimentally via plasmonic resonance shift. This is an ongoing project and is not funded as such, but accommodation for one month period to UTA was financed by fund from Landsvirkjun.

7. Molecular dynamics simulations of vacuum diodes, by Ágúst Valfells, Andrei Manolescu, Kristinn Torfason, and Marjan Ilkov. The optical and field emission of electrons from a cathode, the propagation to the anode, and the space-charge effects are simulated numerically with classical equations of motion where the Coulomb forces between electrons are fully included. The main results in 2014 were on the synchronization of beams released by an array of cathodes and the I-V characteristics of a nanometric diode under field emission. This is an ongoing project, the present funding being based on a Rannis grant.

8. Structural and transport properties of solar cells based on halide-perovskite materials. Participants: Andrei Manolescu, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Charles Goehry. This project is part of 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 project started in June 2014 and Charles Goehry has been hired as a postdoc within this project in November. Atomistic simulations of the structure and transport of optically generated electron-hole pairs are in progress.

9. Fabrication of nano-imprinted resonant structures for thin-film solar cell applications. Participant was Halldór Svavarsson in cooperation with the Nanophotonic Device group at UTA. The project was a part of a doctoral study carried out by a PhD student at UTA (student Tanzina Khaleque, graduated from UTA in summer 2014). The project aimed to design a fast and simple method suitable for a large scale fabrication of periodic 1D and 2D nanostructures for photovoltaic applications. The project was partially funded by grant from Landsvirkjun

Grants and other financial resources

Landsvirkjun, Thermoelectric properties of nanowires, PI Halldór G. Svavarsson, 3.5 million ISK, 2013-2014.

Properties of microscopic vacuum electronic devices, The Icelandic Research Fund, PI Ágúst Valfells, 19.9 million ISK, 2012-2015

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

Travel and other small research funds provided by the School of Science an Engineering were also used.

Main events (visits, presentations, theses, etc.)

16 April: Introduction to the Siesta code for atomistic simulations of nanostructures, talk by Dr. George Alexandru Nemnes from University of Bucharest, Romania, who visited RU within the EEA-Romania academic exchange program.

22 April: Introduction to the R-matrix method for electronic transport calculations, talk by Dr. George Alexandru Nemnes

16 May: Quantum Transport in Core/Shell Nanowires, talk by Prof. Thomas Schäpers, who visited our group also as an examiner of Tómas Örn Rosdahl at his Master thesis presentation which occurred at University of Iceland.

21 August: The Shiba Molecule, talk by Prof. Catalin Pascu Moca from Technical University of Budapest, who visited our group after being an examiner of Thorsten Arnolds at his PhD presentation, at University of Iceland.

19 November: Phase Space Exploration and Synchronization of Arrays of Microdiodes, talk by Marjan Ilkov, Progress Report within his PhD program.

27 November: Spin-orbit torques in ferromagnets and antiferromagnets, talk by Dr. Karel Vyborny from Institute of Physics, Academy of Sciences of the Czech Republic.

18 December: Thesis defense of Abhishek Kumar at Reykjavik University: Theory of non-Markovian dynamics in Fluorescence, supervisor Sigurður Erlingsson.

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

K. Torfason, A. Manolescu, A. Valfells, Molecular Dynamics Simulations of Field Emission From a Planar Nanodiode, arXiv:1412.4537, submitted for publication.

T. Arnold, C.-S. Tang, A. Manolescu, and V. Gudmundsson, Excitation spectra of a quantum ring embedded in a photon cavity, Journal of Optics **17**, 015201 (2015), arXiv:1410.0174.

N. R. Abdullah, C.-S. Tang, A. Manolescu, and V. Gudmundsson, Cavity-photon-switched coherent transient transport in a double quantum waveguide, Journal of Applied Physics, **116**, 233104 (2014), arXiv:1410.4890.

T. Ö. Rosdahl, A. Manolescu, V. Gudmundsson, Signature of snaking states in the conductance of core-shell nanowires, Nano Letters, published online November 26, 2014, arXiv:1409.3429.

M Ilkov, K Torfason, A Manolescu, Á Valfells, Synchronization in arrays of vacuum microdiodes, IEEE Transactions on Electron Devices **62**, 200 (2015), arXiv:1409.0516.

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Coherent transient transport of interacting electrons through a quantum waveguide switch, J. Phys.: Cond. Matt. **27**, 015301 (2015), arXiv:1408.1007.

T. Ö. Rosdahl, A. Manolescu, V. Gudmundsson, Spin and impurity effects on flux-periodic oscillations in core-shell nanowires, Phys. Rev. B **90**, 035421 (2014), arXiv:1404.1798.

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Delocalization of electrons by cavity photons in transport through a quantum dot molecule, Physica E **64**, 254 (2014), arXiv:1403.0382.

V. Gudmundsson, S. Hauksson, A. Johnsen, G. Reinisch, A. Manolescu, C. Besse, G. Dujardin, Excitation of radial collective modes in a quantum dot: Beyond linear response, Annalen der Physik **526**, 235 (2014), arXiv:1311.3252.

A. Manolescu, D. C. Marinescu, T. D. Stanescu, Coulomb interaction effects on the Majorana states in quantum wires, J. Phys.: Cond. Matt. **26**, 172203 (2014), arXiv:1312.3888.

T. Arnold, C.-S. Tang, A. Manolescu, and V. Gudmundsson, Geometry and linearly polarized cavity photon effects on the charge and spin currents of spin-orbit interacting electrons in a quantum ring, European Physics Journal B **87**, 113 (2014), arXiv:1310.5870.

T. Arnold, C.-S. Tang, A. Manolescu, and V. Gudmundsson, Impact of a circularly polarized cavity photon field on the charge and spin flow through an Aharonov-Casher ring, Physica E **60**, 170 (2014), arXiv:1311.3235.

G. Reinish, A. Manolescu, V. Gudmundsson, Coherent nonlinear quantum model for composite fermions, Physics Letters A **378**, 1566 (2014), arXiv:1306.6869.

G. Thorgilsson, G. Viktorsson and S. I. Erlingsson, Recursive Green's function method for multi-terminal nanostructures, Journal of Computational Physics **261**, 256 (2014), arXiv:1305.7363.

S. I. Erlingsson and J. C. Egues, An all electron topological insulator in InAs double wells, arXiv:1312.2034, submitted for publication.

H. G. Svavarsson, S. Einarsson, and A. Brynjolfsdottir, Adsorption applications of unmodified geothermal silica, Geothermics **50**, 30 (2014).

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

Contributions to conferences and other public presentations

A. A. Nila, G. A. Nemnes, A. Manolescu, Ab initio investigation of optical properties in triangular graphene - boron nitride core-shell nanostructures, Conference "Advanced many-body and statistical methods in mesoscopic systems II, September 1-5, 2014, Brasov, Romania, to appear in Romanian Journal of Physics, arXiv:1411.6042.

A. E. Stanciu, G. A. Nemnes, A. Manolescu, Thermoelectric effects in nanostructured quantum wires in the non-linear temperature regime, Conference "Advanced many-body and statistical methods in mesoscopic systems II, September 1-5, 2014, Brasov, Romania, to appear in Romanian Journal of Physics, arXiv:1411.6018.

D. C. Marinescu, A. Manolescu, J. Capps, Anomalous spin and charge Seebeck effect in a quantum well with spin orbit interaction, Proceedings. SPIE 9167, Spintronics VII, 91671M, August 28, 2014; doi:10.1117/12.2063671; http://dx.doi.org/10.1117/12.2063671

M. Ilkov, K. Torfason, A. Manolescu, Á. Valfells, Synchronization of microdiode arrays in the THz band, ICOPS 41, Washington DC, May 25 – 29, 2014, http://www.ece.unm.edu/icops-beams2014/ (poster presentation).

K. Torfason, A. Manolescu, Á. Valfells, Molecular Dynamics Simulations of Field Emission From a Planar Nanodiode and Child Langmuir Current From a Prolate Spheroidal Tip, ICOPS 41, Washington DC, May 25 – 29, 2014, http://www.ece.unm.edu/icops-beams2014/ (poster presentation).

S. I. Erlingsson, An all electrical topological insulator in InAs double wells, in Dirac materials, superconductivity and hybrid structures, Nordita, Stockholm, Sweden, June 16-19 2014, invited talk.

S. I. Erlingsson and J. C. Egues, An all electrical topological insulator in InAs double wells, PASPS-VIII, Washington DC, July 28-30, 2014.

Research plans for 2015

Core-shell nanowires: influence of shell thickness on the conductance of core-shell nanowires; corner localization in shells of polygonal shapes.

Vacuum electronics: electron dynamics at finite temperatures; effects of cathode geometry in nanodiodes with field or photo emission. Comparison of image charge approximation to full Poisson equation solutions for surface field calculation on a hyperbolic spheroid.

Solar cells based on perovskites: alignment of the electric dipoles associated with metylamonium molecules; I-V characteristics under illumination; space-charge effects described by molecular dynamics.

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

Silicon nanowires: Thermal transport properties of silicon nanowires in respect to thermoelectric effects.