

Nanophysics Center, Reykjavik University

Annual Report 2015

Members of the group

The Nanophysics Center (Website nano.ru.is) had the following members during 2015: Five faculty, Andrei Manolescu, Ágúst Valfell, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Gunnar Þorgilsson; two postdoctoral researchers, Kristinn Torfason, and Charles Goehry; one PhD students, Marjan Ilkov.

Visitors: Two undergraduate students, Johannes Krotz and Simon Wozny, from the University of Konstanz stayed at RU did their undergraduate research work at RU, for six months each, on topological insulators. Another undergraduate student, Benjamin Richman, from University of California, Davis, spent at three month at RU working on a research project on rolled up nanowires. Three Master's students from France contributed to the experimental work on Silicon nanowires for three months each.

Main research projects: participants, results, funding

1. Magnetoresistance oscillations in systems with spin-orbit coupling 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 manuscript is in preparation and we are interacting with the experimental group of Prof. Dominik Zumbuhl at the University of Basel who do magnetoresistance measurements which can use our formula to fit their data.
2. Electronic states 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 several graduate students from University of Iceland. The project is part of an ongoing research on time dependent electron transport in nanosystems. The financial support in 2015 was obtained by the collaborator from the research funds of the University of Iceland.
3. Following the initial topological insulator proposal, see Erlingsson and Egues 2015, the same investigators are now looking at extending the proposal to hole based quantum wells. The spin-orbit interaction is usually much stronger in hole systems and we expect that the gap size should increase substantially leading a more experimentally feasible system. The project is still in the early stages. Other topological insulator projects involve Dr. Karel Vyborny from Institute of Physics in Prague. We are studying transport in topological insulators in the presence of magnetic impurities. An undergraduate student, Simon Wozny from the University of Konstanz, is working on this project (he started in October 2015 and will finish in March 2016) under the supervision of SIE. Another related project is on transport in 2D topological insulators-superconductor heterostructures. The results appeared in a bachelor thesis of Johannes Krotz who worked on the project under the supervision of SIE from March to September 2015. The funding for the undergraduate students came from Erasmus Grants.
4. Electronic properties of core-shell nanowires made of semiconductor materials. The participants were Andrei Manolescu and Gunnar Þorgilsson, in cooperation with Anna Sitek and Viðar Guðmundsson from University of Iceland, with Llorens Serra from University of the Balearic Islands (Mallorca) and with Thomas Schäpers from Forschungszentrum Jülich. The main results obtained in 2015 are: optical absorption in multiple domains due to localization of electrons in the corners of a polygonal shell, and

Aharonov-Bohm oscillations of the conductance produced by snaking states created by a magnetic field perpendicular to the nanowire. This is an ongoing project which started in 2012 and still not funded from a grant.

5. Ultra long Silicon nanowires. The participants were Halldór Svavarsson and three MSc.eng. students from France during the summer 2015. The project has two directions: thermoelectrics and photovoltaics. The heat transfer and the optical absorption of arrays of Silicon nanowires were measured recently. The funding is partly provided by Landsvirkjun.

6. Development of plasmonic resonance-based nanophotonic devices. Participant was Halldór Svavarsson in cooperation with the Nanophotonic Device group at University of Texas at Arlington (UTA). The project aims to design simple methods to fabricate periodic nanostructures suitable for sensing applications. This is an ongoing project and is not funded as such, but Halldór regularly visit UTA as a part of the collaboration.

7. Molecular dynamics simulations of vacuum diodes, by Ágúst Valfell, 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 2015 were on the robustness of the charge bunching at finite temperatures of the cathode and on the I-V characteristics of a nanometric diode under field emission. The funding in 2015 was based on a Rannis grant.

8. Structural and transport properties of solar cells based on halide-perovskite materials. Main participants: Andrei Manolescu, Charles Goehry, Kristinn Torfason, and Marjan Ilkov. This project (acronym Perpfect) 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. Atomistic simulations of $\text{CH}_3\text{NH}_3\text{-PbI}_3$ were carried out by Charles Goehry and continued by Kristinn Torfason. Kristinn adapted his molecular dynamics code to the transport of optically generated electron-hole pairs and implementation of dipole moments is now in progress.

Grants and other financial resources

Properties of microscopic vacuum electronic devices, The Icelandic Research Fund, PI Ágúst Valfell, 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.

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

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

12-20 February, visit of Blazej Jaworowski, PhD student at Wroclaw University of Technology, funded by Erasmus.

18 February, Fractional Chern Insulator on Lieb lattice, talk by Blazej Jaworowski.

20 February – 4 March, visit of Maciej Bieniek, PhD student at Wroclaw University of Technology, funded by Erasmus.

20 May, Collective behavior of molecular dipoles in $\text{CH}_3\text{NH}_3\text{PbI}_3$, talk by Charles Goehry from RU.

2-14 September, visit of George Alexandru Nemnes from University of Bucharest, related to the Perpfect project.

27 September – 9 October, visit of Neculai Plugaru, from National Institute for Materials Science, Bucharest, related to the Perpfect project.

12 October, Thesis defense of Marjan Ilkov at Reykjavik University: Space-charge dynamics in microdiodes, supervisor Ágúst Valfells.

14 October, Biological Manipulation with Intense Electromagnetic Radiation, talk by Allen Garner from Purdue University.

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

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, [arXiv:1512.00392](https://arxiv.org/abs/1512.00392) (2015).

A. Sitek, G. Thorgilsson, V. Gudmundsson, A. Manolescu, Multi-domain electromagnetic absorption of triangular quantum rings, submitted to publication, [arXiv:1511.05596](https://arxiv.org/abs/1511.05596) (2015).

G. A. Nemnes, C. Goehry, T. L. Mitran, A. Nicolaev, L. Ion, S. Antohe, N. Plugaru, A. Manolescu, Band alignment and charge transfer in rutile- $\text{TiO}_2/\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$ interfaces, *Physical Chemistry Chemical Physics (PCCP)* **17**, 30417 (2015).

M. Ilkov, K. Torfason, A. Manolescu, A. Valfells, Terahertz pulsed photogenerated current in microdiodes at room temperature, *Applied Physics Letters*, **107**, 203508 (2015) [arXiv:1508.06308](https://arxiv.org/abs/1508.06308).

B. Jaworowski, A. Manolescu, P. Potasz, Fractional Chern Insulator phase at the transition between checkerboard and Lieb lattice, *Phys. Rev. B* **92**, 245119 (2015), [arXiv:1508.04399](https://arxiv.org/abs/1508.04399).

C. Goehry, G. A. Nemnes, A. Manolescu, Collective Behavior of Molecular Dipoles in $\text{CH}_3\text{NH}_3\text{PbI}_3$, *J. Phys. Chem. C* **119**, 19674 (2015).

N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Gudmundsson, Cavity-photon controlled thermoelectric transport through a quantum wire, submitted to publication, [arXiv:1507.06574](https://arxiv.org/abs/1507.06574) (2015).

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, submitted to publication, [arXiv:1506.02993](https://arxiv.org/abs/1506.02993) (2015)

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*, DOI: 10.1002/andp.201500298, [arXiv:1505.03181](https://arxiv.org/abs/1505.03181) (2015)

- A. Sitek, L. Serra, V. Gudmundsson, A. Manolescu, Electron localization and optical absorption of polygonal quantum rings, *Phys. Rev. B* **91**, 235429 (2015), [arXiv:1503.09186](#).
- S. I. Erlingsson, A. Manolescu, D. C. Marinescu, Asymmetric Landau bands due to spin-orbit coupling, *J. Phys.: Condens. Matter* **27**, 225303 (2015), [arXiv:1504.04699](#).
- V. Gudmundsson, A. Sitek, P.-Y. Lin, N. R. Abdullah, C.-S. Tang, A. Manolescu, Coupled collective and Rabi oscillations triggered by electron transport through a photon cavity, *ACS Photonics* **2**, 930 (2015), <http://pubs.acs.org/doi/abs/10.1021/acsp Photonics.5b00115>, [arXiv:1502.06242](#).
- J. Capps, D. C. Marinescu, A. Manolescu, Coulomb interaction effects in a two dimensional quantum well with spin-orbit interaction, *Phys. Rev. B* **91**, 165301 (2015).
- K. Torfason, A. Manolescu, A. Valfells, Molecular Dynamics Simulations of Field Emission From a Planar Nanodiode, *Physics of Plasmas* **22**, 033109 (2015), [arXiv:1412.4537](#).
- A. A. Nila, G. A. Nemnes, A. Manolescu, Ab initio investigation of optical properties in triangular graphene - boron nitride core-shell nanostructures, *Romanian Journal of Physics* **60**, 696 (2015), [arXiv:1411.6042](#).
- A. E. Stanciu, G. A. Nemnes, A. Manolescu, Thermoelectric effects in nanostructured quantum wires in the non-linear temperature regime, *Romanian Journal of Physics* **60**, 716 (2015), [arXiv:1411.6018](#).
- 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](#).
- T. Ö. Rosdahl, A. Manolescu, V. Gudmundsson, Signature of snaking states in the conductance of core-shell nanowires, *Nano Lett.* **15**, 254 (2015), DOI: 10.1021/nl503499w, [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](#).
- Sigurdur I. Erlingsson and J. Carlos Egues, All-electron topological insulator in InAs double wells, *Phys. Rev. B* **91**, 035312 (2015).
- Halldor Gudfinnur Svavarsson, Birgir Hrafn Hallgrímsson, Manoj Niraula, Kyu Jin Lee, Robert Magnusson, Large arrays of ultra-high aspect ratio periodic silicon nanowires obtained via top-down route, accepted for publication in *Applied Physics A: Materials science and processing* (2015).
- Johannes Krotz, Quantum Transport in Topological Insulator – Superconductor Heterostructures, Bachelorarbeit, Universität Konstanz, (2015) – Supervised by Sigurdur Erlingsson.

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

Contributions to conferences and other public presentations

G. A. Nemnes, C. Visan, A. Manolescu, Novel phononic-crystal design by tailored graphene-like materials, 4-th Nano Today Conference, Dubai 6-10 December 2015, <http://www.nanotoday-conference.com/>

A. Loveless, A. Garner, A. Valfells, Unifying Paschen curve conditions across pressure and gap distance, 57th Annual Meeting APS-DPP, Savannah, Georgia, 16-20 November 2015, <https://www.aps.org/units/dpp/meetings/annual/>

N. Plugaru, G. A. Nemnes, L. Filip, A. Manolescu, Atomistic simulations of methylammonium lead halide layers on PbTiO₃, Psi-k, San Sebastian 6-10 September 2015, <http://nano-bio.ehu.es/psik2015/>

A. Sitek, V. Gudmundsson, A. Manolescu, Symmetry dependent electron localization and optical absorption of polygonal quantum rings, ICTON 2015 Budapest, IEEE Xplore Digital Library, DOI: [10.1109/ICTON.2015.7193541](https://doi.org/10.1109/ICTON.2015.7193541) , [arXiv:1505.00207](https://arxiv.org/abs/1505.00207) (2015).

C. Besleaga, V. Stancu, A. G. Tomulescu, M. Sima, L. M. Trinca, G. E. Stan, A.C. Galca, L. Pintilie, I. Pintilie, A. Radu, S. Iftimie, L. Ion, S. Antohe, A. Nemnes, C. Goehry, A. Manolescu, Hybrid perovskite solar cells: aging effects and Reliability, ROCAM, Bucharest, 7-10 July 2015, <http://rocam.unibuc.ro/rocam2015/index.php>

M. Ilkov, K. Torfason, A. Manolescu, Á Valfells, Thermal effects in microdiode bunching, ICOPS 42, Antalya, 24 – 28 May, 2015. <http://ece-events.unm.edu/icops2015/>

A. Manolescu, Magnetoresistance of core-shell nanowires, Nanocontrol Network Meeting, Aarhus 14-16 January 2015. <http://butler.cc.tut.fi/~rasanene/norden/>

Halldor G. Svavarsson, Hronn Arnardottir, Albert Albertsson, Asa Brynjolfsdottir, Application of unmodified geothermal silica for protein extraction, World Geothermal Congress, Melbourne, Australia, 19.-24. April 2015

Hronn Arnardottir, Asa Brynjolfsdottir, Albert Albertsson, Halldor G. Svavarsson, Biomass production using geothermal flue gas at the Blue Lagoon, Iceland, World Geothermal Congress, Melbourne, Australia, 19.-24. April 2015

Halldor. G. Svavarsson, Hronn Arnardottir, Asa Brynjolfsdottir, Lipid content in Blue-green algae fed on geothermal flue-gas at Blue Lagoon, Iceland, 28. Nordic Lipidforum Symposium, Reykjavik, Iceland, 3.-6. 2015

Research plans for 2016

High photoconductive oxide films functionalized with GeSi nanoparticles for environmental applications (PhotoNanoP): M-ERA.NET project accepted for funding in 2015, to begin in 2016. Participants: Halldór Svavarsson, Sigurður Erlingsson, Andri Manolescu. A PhD student will be recruited..

Core-shell nanowires: Thermoelectric transport, Majorana states, Coulomb effects.

Vacuum electronics: Effects of cathode geometry in nanodiodes with field or photo emission. Design and inception of experiment on THz generation (depending on funding). Coherent control of ultrafast laser induced emission and its application for a coherent light source (depending on funding). Modified Paschen curves at high pressure and gap spacing.

Solar cells based on perovskites: interface halid-perovskite with a ferroelectric, polarization and hysteresis; 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
Photovoltaic application 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)