Nanophysics Center, Reykjavik University
Annual Report 2021

Members of the group

In 2021 The Nanophysics Center (website nano.ru.is) had four full time faculty staff, Andrei Manolescu, Ágúst Valfells, Halldór Svavarsson, Sigurður Ingi Erlingsson, plus Gunnar Þorgilsson who is at ISOR, but still partly affiliated with us. Four other members were postdoctoral researchers Anna Sitek, Kristinn Torfason, Muhammad Taha Sultan, and Movaffaq Kateb. Taha has also been affiliated with University of Iceland, and Movaffaq moved to Chalmers University (Sweden) in July. The group included several PhD students who started their program earlier, Kristján Óttar Klausen, Hadi Rezaie, Hamed Gramizadeh, Hákon Örn Árnason, and Elham Aghabalaei Fakhri. Two new PhD students joined the group Rachel Elizabeth Brophy in August (former Master student with us), and Yuan Zhou in October. Three BS students worked on research projects with us, Þorsteinn Hanning Kristinsson, Brynjar Ingi Óðinsson, and Freyr Hlynsson.

Main research projects: participants, results, work in progress

Thermoelectric transport in core-shell nanowires.
This is a Rannis funded project where Hadi and Movaffaq calculated the heat transported by semiconductor nanowires using the software LAMMPS. Their results suggest that the transversal geometry of the nanowires is important for heat transport. They showed that the triangular cross section is more favorable to heat transport along the nanowire than other geometries, for nanowires with 5-20 nm diameters and several hundreds of nm length. They also analyzed tubular nanowires, and also core-shell nanowires based on silicon and germanium and compared the results. Again, the triangular geometry is more heat conductive. The results were sent to the publication and they are now under review. Separately, Movaffaq calculated the melting temperatures of core-shell nanoparticles and nanowires based on copper oxide, using molecular dynamics simulations. He also performed a methodological study of the effect of the Coulomb forces on the deposition of copper thin layers, published in Surface & Coatings Technology.

Spin-orbit interaction in core-shell nanowires
We began an implementation of the k·p and Schrödinger-Poisson methods to obtain the spin-orbit interaction in a tubular nanowire of a polygonal geometry. The method includes the external electric field created with gates in contact with the nanowire surface. The model includes material parameters, such as the band and spin-orbit gaps. The Coulomb interaction between the electrons is included in the Poisson equation, which is similar to Hartree approximation. 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. In this moment the code is under tests.

Majorana states in core-shell prismatic nanowires.
The PhD student Kristján Óttar Klausen made progress in computing the quantum states of states of a semiconductor shell of a core-shell nanowire with asymmetric induced superconductivity, exploring radial, angular and longitudinal asymmetry. With parametric increase of the asymmetry, the gradual breakdown of the induced superconducting gap has been studied. By exploring the electron-hole coherence within the semiconducting part of the shell, the Andreev reflection model of the proximity

effect is confirmed for the lowest energy values. Using geometric algebra, various mathematical relations fundamental to the theory of Majorana Zero Modes have been studied, such as the gauge field formulation of spin-orbit coupling and its relation to non-Abelian exchange statistics. Currently two manuscripts on these subjects are in construction.

Atomistic calculations of 2D materials.
Andrei Manolescu participated in a project on structural properties of two dimensional materials derived by atomistic calculations, led by Nzar Rauf Abdullah from University of Sulaimani (Iraq). The studied materials were graphene and silicene based codoped with B and N. The focus is on the mechanical, thermoelectrical, and optical properties of these materials.

Halide-perovskite materials for photovoltaic applications
This is a EEA funded project in collaboration with a group from National Institute for Materials Physics, Romania, and another group from University of Oslo. The master student Rachel Brophy and the postdoctoral researcher Movaffaq Kateb studied the migration of Iodine ions in the perovskite material $CH_3NH_3PbI_3$ (MAPI) using molecular dynamics simulations of the lattice dynamics using the LAMMPS software. The goal is to describe the degradation of the MAPI material used for solar cells. The simulations include the presence of grain boundaries and internal electric fields. In parallel Kristinn Torfason performed another series of calculations, of the electronic states and band alignment at the interface between MAPI and a hole transporter layer based on copper oxide, with the goal of describing the effect of atom vacancies near the interface. He uses the DFT method and the Siesta software. Rachel Brophy has also started experimental work on preparing MAPI based solar cells in the lab, under the supervision of a specialist from Romania, Dr. Ioana Vlaicu.

Piezoresistance of Silicon nanowires.
The doctoral student Elham Aghabalaei Fakhri, supervised by Halldór Svavarsson and Snorri Ingvarsson at UI, made significant progress in this project. Disordered arrays of silicon nanofibers and nanowires with 20-50 nm diameter and up to several μm in length were obtained by top-down etching. A variation of the electrical resistance in the presence of stress induced by a blown gas was obtained. The results are promising, but the control of the gas blow, and the quality of the electrical contacts between metallic electrodes and the nanowires still need to be improved. Experiments with uniaxial load also gave promising result and a manuscript for a journal paper is now in preparation.

Electronic properties of vacuum diodes.
Kristinn Torfason is studying surface inhomogeneities using the molecular dynamics code. He is currently studying emission from an emitter surface made of lanthanum hexaboride-Vanadium Diboride (LaB6-VB2). He is comparing his results with experimental data. Brynjar Ingi Óðinsson used the MD code to run simulations with ions and experimented with adding recombination effects for the ions. The results look promising and have generated a lot of discussion about how to implement recombination in the MD code. A new doctoral student Yuan Zhou was hired with a grant from RU. She arrived at the end of October and started by familiarizing herself with our previous work and the MD code. The first part of her project will be to study the emission from carbon nanotubes. The doctoral student Hákon Örn Árnasson performed simulations of the photoemitted current due to a short laser pulse with a Gaussian time profile. The goal is to describe the space-charge effects on the electrical pulse and Ramo current. In 2021 we also studied the effect of increased emission at the edges of finite-size cathodes on the current-temperature characteristics of thermionic cathodes, known as Miram curves. The thermionic cathodes emit in three regimes: the source-limited regime, the space-charge-limited regime and the transition range refereed to as a “knee”. In the case of infinite emitters the transition between the source-limited and space-charge-limited emission is abrupt, while the finite-size cathodes show a smooth “knee”. We compared the Miram curves obtained from square emitters of different size and showed that the transition range becomes smoother with decreasing emitting area. Next we studied separately the contributions from narrow areas at the edges of

the cathodes and from the remaining internal parts. The shape of the latter contribution does not depend on the emitter size and resembles the one of infinite systems, while the edge current increase slows down considerably with decreasing emitting area. This confirms that the shape in the "knee" is determined by the emission from the edges. These results were published in Physical Review Applied 16, 034043 (2021)

Grants and other financial resources

Thermoelectric transport in core-shell nanowires, The Icelandic Research Fund, Andrei Manolescu and Sigurdur Ingi Erlingsson, 51.1 mil. ISK (2019-2022)

A possible basis for quantum computation: Majorana zero modes in tubular nanowires, The Icelandic Research Fund, doctoral grant, Kristján Óttar Klausen, 13 mil. ISK (2020-2022).

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 three PhD students, Elham Aghabalaei Fakhri, Hamed Gramizadeh, and Yuan Zhou were provided by the research funds of Reykjavik University, the positions being obtained in 2020, 2018, and 2021, respectively.

Fund for a postdoc for 2 years. Postdoc Abduk Rahman Mallah has been hired and is expected to Iceland in few weeks. EEA funded project on a novel way to produce solar-grade silicon by using by-product from aluminum smelters. Acronym SiSal-Pilot. Led by NTNU in Norway. Halldór Svavarson together with Gudrun Saevarsdottir are responsible for the Icelandic part. Total grant for the Icelandic activity is 298.000 euros (~45 million ISK)

Funds for three summer BS students were obtained from The Directorate of Labor (Vinnumálastofnun), via Reykjavik University.

The Master and further PhD student Rachel Brophy was funded by Landsvirkjun and PERLA-PV.

Events related to the activity of the center (short visits, presentations, theses, etc.) were severely limited due to the Covid related crisis

25 May, Master student Rachel Elizabeth Brophy defends her thesis entitled "Computer simulations of ionic diffusion in MAPI perovskites". Supervisors Andrei Manolescu and Halldór Svavarsson, examiner Professor Hannes Jónsson from University of Iceland.

24 August, Sigurdur Erlingsson and Andrei Manolescu talked about recent projects and collaboration possibilities at an online Nordita meeting.

23 September, Dr. Charles Eddy, Science Director for Europe of US Office of Naval Research Global, visited the group and discussed funding mechanisms and future possible projects.

3-15 October, Dr. Ioana Vlaicu, chemist expert from National Institute of Materials Physics, Romania, visited the group and instructed PhD student Rachel Brophy and Dr. Taha Sultan, on the preparation of MAPI perovskite samples for solar cells.

11 November, Dr. Habib Rostami from Nordita visited the group and discussed a cooperation plan on nanowires with polygonal cross section.

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

N. R. Abdullah, B. J. Abdullah, H. O. Rashid, C.-S. Tang, A. Manolescu, V. Gudmundsson, Enhanced electronic and optical responses of Nitrogen- or Boron-doped BeO monolayer: First principle computation, accepted for publication in Superlattices and Microstructures, arXiv:2108.12912 (2021).

N. Filipoiu, T. L. Mitran, D. V. Anghel, M. Florea, I. Pintilie, A. Manolescu, G. A. Nemnes, Machine learning aided investigation of opto-electronic properties and stability of mixed-cation mixed-halide perovskite materials, Energies **14**, 5431 (2021).

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, submitted for publication, arXiv:2108.00387 (2021).

A. Sitek, K. Torfason, A. Manolescu, A. Valfells, Edge effect on the current-temperature characteristic of thermionic cathodes, Phys. Rev. Applied **16**, 034043 (2021), arXiv:2106.05311 .

M. Urbaneja Torres, K. O. Klausen, A. Sitek, S. I. Erlingsson, V. Gudmundsson, A. Manolescu, Anisotropic electromagnetic field emitted by core-shell semiconductor nanowires driven by an alternating current, J. Appl. Phys. **130**, 034301 (2021) arXiv:1912.10284.

M. T. Sultan, H. Ö. Árnason, M. K. Kateshamshir, A. Manolescu, H. G. Svavarsson, Á. Valfells, Enhanced photoemission from surface modulated GaAs:Ge, Nano Select 2021, **1** (2021) https://doi.org/10.1002/nano.202100012.

N. R. Abdullah, M. T. Kareem, H. O. Rashid, A. Manolescu, V. Gudmundsson, Spin-polarized DFT modeling of electronic, magnetic, thermal and optical properties of silicene doped with transition metals, Physica E **129**, 114644 (2021) arXiv:2009.14804**.**

N. R. Abdullah, H. O. Rashid, C.-S. Tang, A. Manolescu, V. Gudmundsson, Role of interlayer spacing on electronic, thermal and optical properties of BN-codoped bilayer graphene: Influence of the interlayer and the induced dipole-dipole interactions, Journal of Physics and Chemistry of Solids **155**, 110095 (2021), arXiv:2102.09543.

M. Kateb, J. T. Gudmundsson, P. Brault, A. Manolescu, S. Ingvarsson, On the role of ion potential energy in low energy HiPIMS deposition: An atomistic simulation, accepted for publication is Surface & Coatings Technology (2021) arXiv:2101.05896 .

K. Torfason, A. Sitek, A. Manolescu, Á. Valfells, Dynamics of a Field Emitted Beam from a Microscopic Inhomogeneous Cathode, IEEE Transactions on Electron Devices **68**, 2461 (2021) arXiv:2011.13731.

A. Sitek, K. Torfason, A. Manolescu, and A. Valfells, Space-charge effects in the field-assisted thermionic emission from nonuniform cathodes, Physical Review Applied **15**, 014040 (2021) (selected as an Editors' Suggestion), arXiv:2009.13616 .

V. Gudmundsson, N. R. Abdullah, C.-S. Tang, A. Manolescu, V. Moldoveanu, Self-induction and magnetic effects in electron transport through a photon cavity, Physica E 127 (2021) 114544 (2021), arXiv:2005.10914.

N. R. Abdullah, H. O. Rashid, C.-S. Tang, A. Manolescu, V. Gudmundsson, Properties of BSi_6N monolayers derived by first-principle computation, Physica E **127**, 114556 (2021), arXiv:2008.03782.

J. B. Gunnarsson, K. Torfason, A. Manolescu, A. Valfells, Space-Charge Limited Current from a Finite Emitter in Nano- and Microdiodes, IEEE Transactions on Electron Devices **68**, 342 (2021), arXiv:2010.01334 .

Aleš Cahlík, Jack Hellerstedt, Jesús I Mendieta-Moreno, Martin Švec, Vijai M Santhini, Simon Pascal, Diego Soler-Polo, Sigurdur I Erlingsson, Karel Výborný, Pingo Mutombo, Ondrej Marsalek, Olivier Siri, Pavel Jelínek Significance of nuclear quantum effects in hydrogen bonded molecular chains, ACS Nano **15**, 10357 (2021)

Simon Wozny, Martin Leijnse, and Sigurdur I. Erlingsson, Dynamic impurities in two-dimensional topological-insulator edge states, Phys. Rev. B **104**, 205418 (2021)

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

Contributions to conferences

N. Filipoiu, T.L. Mitran, D.V. Anghel, M. Florea, I. Pintilie, A. Manolescu, G. A. Nemnes, Prediction of electronic properties and stability assessment of mixed-cation mixed-halogen perovskite materials using artificial neural networks, MATERIALS, METHODS & TECHNOLOGIES, 24th International Conference, 19-22 August 2022, Burgas, Bulgaria

G.A. Nemnes, T.L. Mitran, A.T. Preda, D.V. Anghel, I. Ghiu, V. Baran, M. Marciu, A. Manolescu, Mapping energy spectra of Coulomb interacting bi-particle systems using multi-target regression methods, Mathematical Modeling in Physical Sciences September 6-9, 2021 Virtual, on-line Conference (IC-MSQUARE)

E. Fakhri, M. T. Sultan, A. Manolescu, S. Ingvarsson, N. Plugaru, R. Plugaru, H. G. Svavarsson, Synthesis and photoluminescence study of silicon nanowires obtained by metal assisted chemical etching, 2021 International Semiconductor Conference (CAS) Romania, DOI: 10.1109/CAS52836.2021.9604178, https://ieeexplore.ieee.org/document/9604178

M. T. Sultan, J. T. Gudmundsson, A. Manolescu, M. L. Ciurea, H. G. Svavarsson, S. Ingvarsson Photoluminescence study of Si1-xGex nanoparticles in various oxide matrices, 2021 International Semiconductor Conference (CAS) Romania, DOI: 10.1109/CAS52836.2021.9604131 , https://ieeexplore.ieee.org/abstract/document/9604131

M. T. Sultan, H. Ö. Árnason, S. Ingvarsson, U. B. Arnalds, H. G. Svavarsson, A. Manolescu, A. Valfells

Facile formation of self-assembled Ga droplets on GaAs (001) substrate, 2021 International Semiconductor Conference (CAS) Romania, DOI: 10.1109/CAS52836.2021.9604129, https://ieeexplore.ieee.org/abstract/document/9604129

Research plans for 2022

Drag phonon drag effect and heat conduction of nanowires.

Piezoresistance and other stress effects in arrays of Silicon nanofibers and nanowires.

Molecular dynamics of perovskite materials for photovoltaics applications.

Proximity induced superconductivity in tubular semiconductor nanowires.

Spin-orbit coupling in core-shell nanowires.

Transport in topological nanowires.

Field emission from carbon nanotubes and carbon fibers.