

# Nanophysics Center, Reykjavik University

## Annual Report 2022

### Members of the group

During 2022 our group (website [nano.ru.is](http://nano.ru.is) or <https://en.ru.is/nano>) had five full time faculty staff: Andrei Manolescu, Ágúst Valfell, Halldór Svavarsson, Sigurður Ingi Erlingsson, and Kristinn Torfason. Gunnar Þorgilsson and Muhammad Taha Sultan were external collaborators, but still partly affiliated with us. Abdul Raman Mallah was a full-time postdoctoral scientist. Anna Sitek, from Wroclaw University (Poland) and Movaffaq Kateb from Chalmers University (Sweden) were close collaborators on two separate projects. The group included several PhD students: Kristján Óttar Klausen, Hadi Rezaie Heris, Hamed Gramizadeh, Hákon Örn Árnason, Elham Aghabalaei Fakhri and Rachel Elizabeth Brophy, and Yuan Zhou. Three BS students continued to work on research projects with us, Þorsteinn Hanning Kristinsson, Brynjar Ingi Óðinsson, and Freyr Hlynsson. Three guest doctoral students from Romania visited the group for two months (October-November) and worked with us on collaborative projects: Amanda Preda, Nicolae Filipoiu, and Ioan Ghitu.

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

#### *Thermoelectric transport in core-shell nanowires.*

This research was performed under a Rannis project obtained by Hadi, for an extension to a fourth year of his doctoral program. Hadi's project was in continuation of a previous Rannis project led by Andrei, which was financially closed at the end of 2021. Hadi calculated the thermoelectric and heat currents associated with electrons in semiconductor nanowires with polygonal cross sections, using the Green's function method. The results were presented to the International Conference of Semiconductors in Romania and appeared in the corresponding IEEE Proceedings (as a 4-page paper). A more extended manuscript including the effect of impurities was sent for publication at the end of the year. He also began a new series of calculations concerning the effect of phonons on the thermoelectric currents in nanowires, known as the phonon drag effect.

#### *Proximity induced superconductivity in core-shell prismatic nanowires.*

The PhD student Kristján Óttar Klausen successfully defended his PhD thesis on this subject. His work covered the electron-hole coherence in a proximitized nanowire, the effect of the spin-orbit interaction and of an external magnetic field. In particular, he obtained interesting results on the oscillations of the electron-like and hole-like wave functions in the presence of a magnetic field. The results were appreciated by our collaborators from Forschungszentrum Jülich (Germany) and Riken Tokyo (Japan) where experimental work on this topic is performed.

#### *Spin-orbit interaction in core-shell nanowires*

Anna Sitek made significant progress with implementing the  $k \cdot p$  method to obtain the spin-orbit interaction in tubular nanowires of a polygonal geometry. The  $k \cdot p$  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. She got the first results in the second part of 2023, showing that the spin-orbit effect of Rashba type decreases with decreasing the shell thickness. A manuscript on this subject is in progress.

#### *Spin-orbit effect on the magnetoresistance of 2D systems*

This project was funded by the Reykjavik University Research Fund and it is a collaboration between groups at the University of Sao Paulo, Sao Carlos, Iowa University and the University of Basel. The funding was used to pay salaries for doctoral student Hamed Gramizadeh, who is expected to defend his thesis in spring 2023. The goal of the project was to obtain methods to extract values of spin-orbit parameters from experimental data – namely Shubnikov-de Haas oscillations. Publications are in final stages of preparation, and will be submitted prior to defense date.

#### *Halide-perovskite materials for photovoltaic applications*

This is an EEA funded project in collaboration with a group from National Institute for Materials Physics, Romania, and another group from University of Oslo. The doctoral student Rachel Brophy and the postdoctoral researcher Movaffaq Kateb finalized a computational study on the migration of Iodine ions in the perovskite material  $\text{CH}_3\text{NH}_3\text{PbI}_3$  (MAPI) using molecular dynamics simulations with the LAMMPS software. They showed that the iodine vacancy has a higher mobility than the iodine interstitial ion, and that both mobilities decrease when a pressure is applied to the lattice. This effect suggests that the iodine migration in MAPI may be reduced in the presence of stress. In parallel Kristinn Torfason continued his calculations of the electronic states and band alignment at the interface between MAPI and a layer of copper and nickel oxide, with the goal of describing the effect of atom vacancies near the interface. He uses the DFT method and the Siesta software.

#### *Piezoresistance of Silicon nanowires.*

This was the main work of the doctoral student Elham Aghabalaei Fakhri, supervised by Halldór Svavarsson at RU and Snorri Ingvarsson at UI. The main achievement in 2023 was the discovery that these nanowires are so sensitive to pressure variation that they can be used as a sensor of human breath. A paper describing this sensor behavior was presented at the International Conference of Semiconductors in Romania and appeared in the corresponding IEEE Proceedings (as a 4-page paper). A more extended manuscript is in progress. In the manuscript we make the hypotheses that the effectiveness of the sensor may be attributed both to piezoresistance and humidity in the breath. Abdul Raman Mallah is going to use Comsol to model I-V characteristics of different metal electrodes on the breath-sensing devices.

#### *Electronic properties of vacuum diodes.*

The doctoral student Yuan Zhou performed a series of calculations using the COMSOL software, on the electric field at the surface of a carbon nanofiber in the presence of a point charge situated in the neighborhood of the surface. The intention was to evaluate the effects of the image charge for selected positions of the electron, and subsequently to use a machine learning method to calculate the field when the electron is situated at other locations. The doctoral student Hákon Örn Árnasson continued his simulations of the photoemitted current due to a short laser pulse, and finalized his PhD thesis which was successfully defended in the second week of 2023.

### **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).

Geometry effect on phonon drag in core-shell nanowires, The Icelandic Research fund, doctoral grant, Hadi Rezaie Heris, 6.5 mil. ISK (2021-2022).

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 the PhD students Elham Aghabalaei Fakhri, Hamed Gramizadeh, Yuan Zhou, and Rachel Brophy were provided by the research funds of Reykjavik University.

The postdoctoral researcher Abdur Rahman Mallah has been funded by the EEA project called SiSal-Pilot, on a novel way to produce solar-grade silicon by using by-product from aluminum smelters Acronym SiSal-Pilot.

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

21-23 January, Dr. Andrew Greenwood, from Air Force Office of Scientific Research, visited our group and discussed possibilities of future funding for the computer simulations of vacuum electronic devices. Following his visit, we submitted a new research proposal.

27 May, Andrei Manolescu and Rachel Brophy, visit at National Institute of Materials Physics, Romania, partners in the PERLA-PV project, for two weeks each.

28 July, Andrei Manolescu, talk at Forschungszentrum Jülich (Germany), Thomas Schäpers group, entitled "Localization of electrons and Majorana states in tubular semiconductors"

30 September, Kristján Klausen defended his PhD thesis entitled "Majorana Zero Modes in Tubular Nanowires", with external examiner Dr. Habib Rostami.

12-15 October, Northern Lights Conference on spin, topology, and superconductivity, held at National Museum of Iceland, organized by Next Generation Partnership Network of the Universität Hamburg, with the help of local organizers Andrei Manolescu, Sigurður Ingi Erlingsson, and Vidar Gudmundsson.

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

T. L. Mitran, R. E. Brophy, M. Cuzminschi, N. Filipoiu, M. Kateb, I. Pintilie, A. Manolescu, G. A. Nemnes, Ab Initio Studies on perovskites, Chapter 5 in the book Low-Dimensional Halide Perovskites: Structure, Synthesis, and Applications, Edited by Y. Zhan, M. Khalid, and N. Arshid, Elsevier <https://doi.org/10.1016/B978-0-323-88522-5.00012-0> ISBN: 978-0-323-88522-5 (2022).

N. Filipoiu, Anca G. Mirea, Sarah Derbali, C. -A. Pantis-Simut, D. -V. Anghel, A. Manolescu, Ioana Pintilie, Mihaela Florea, G. A. Nemnes, Optoelectronic and stability properties of quasi-2D alkylammonium based perovskites, accepted for publication at Physical Chemistry Chemical Physics, [arXiv:2210.04596](https://arxiv.org/abs/2210.04596) (2022).

K. O. Klausen, A. Sitek, S. I. Erlingsson, A. Manolescu, Flux-periodic oscillations in proximitized core-shell nanowires, submitted for publication, [arXiv:2209.13076](https://arxiv.org/abs/2209.13076) (2022).

N. Filipoiu, A. T. Preda, D. V. Anghel, R. Patru, R. E. Brophy, M. Kateb, C. Besleaga, A. G. Tomulescu, I. Pintilie, A. Manolescu, G. A. Nemnes, Capacitive and inductive effects in perovskite solar cells: the

different roles of ionic current and ionic charge accumulation, Phys. Rev. Applied 18, 064087 (2022), [arXiv:2208.10199](https://arxiv.org/abs/2208.10199) .

E. Fakhri, R. Plugaru, M. T. Sultan, T. H. Kristinsson, H. Ö. Árnason, N. Plugaru, A. Manolescu, S. Ingvarsson, H. G. Svavarsson, Piezoresistance characterization of silicon nanowires in uniaxial and isostatic pressure variation, Sensors 22, 6340 (2022), [arXiv:2206.04991](https://arxiv.org/abs/2206.04991).

R. Plugaru, E. Fakhri, C. Romanitan, I. Mihalache, G. Craciun, N. Plugaru, H. O. Arnason, M. T. Sultan, G. A. Nemnes, S. T. Ingvarsson, H. G. Svavarsson, A. Manolescu, Structure and electrical behavior of silicon nanowires prepared by MACE process, Surfaces and Interfaces 33, 102167 (2022), [arXiv:2206.05006](https://arxiv.org/abs/2206.05006) .

V. Gudmundsson, V. Mughnetsyan, N. R. Abdullah, C.-S. Tang, V. Moldoveanu, A. Manolescu, Effects of a far-infrared photon cavity field on the magnetization of a square quantum dot array, submitted for publication, Phys. Rev. B 106, 115308 (2022) [arXiv:2203.11029](https://arxiv.org/abs/2203.11029) .

G. A. Nemnes, T. L. Mitran, A. T. Preda, V. V. Baran, D. V. Anghel, I. Ghiu, M. Marciu, A. Manolescu, Investigation of bi-particle states in gate-array-controlled quantum-dot systems aided by machine learning techniques, Physica Scripta 97, 055813 (2022), [arXiv:2203.14398](https://arxiv.org/abs/2203.14398).

H. Rezaie Heris, M. Kateb, S. I. Erlingsson, and A. Manolescu, Effects of transverse geometry on the thermal conductivity of Si and Ge nanowires, Surfaces and Interfaces 30, 101834 (2022), [arXiv:2203.15596](https://arxiv.org/abs/2203.15596).

V. Gudmundsson, V. Mughnetsyan, N. R. Abdullah, C.-S. Tang, V. Moldoveanu, A. Manolescu, Unified approach to cyclotron and plasmon resonances in a periodic 2DEG hosting the Hofstadter butterfly, Phys. Rev. B 105, 155302 (2022), [arXiv:2112.08216](https://arxiv.org/abs/2112.08216).

B. R. Pirot, N. R. Abdullah, A. K. Ahmeda, A. Manolescu, V. Gudmundsson, Thermal transport controlled by intra- and inter-dot Coulomb interactions in sequential and cotunneling serially-coupled double quantum dots, Physica B 629, 413646 (2022) [arXiv:2201.00121](https://arxiv.org/abs/2201.00121).

N. R. Abdullah, H. O. Rashid, C.-S. Tang, A. Manolescu, V. Gudmundsson, Controlling physical properties of bilayer graphene by stacking orientation caused by interaction between B and N dopant atoms, Material Science & Engineering B 276, 115554 (2022), [arXiv:2101.00462](https://arxiv.org/abs/2101.00462).

M de Witt, Á Valfells, JN Larsen, H Stefánsson, Simulation of pathways toward low-carbon electricity generation in the Arctic, Sustainability 14 (22), 15311 (2022).

Samuel Warren Scott, Léa Lévy, Cari Covell, Hjalti Franzson, Benoit Gibert, Ágúst Valfells, Juliet Newson, Julia Frolova, Egill Júlíusson, María Sigríður Guðjónsdóttir, Valgarður: A Database of the Petrophysical, Mineralogical, and Chemical Properties of Icelandic Rocks Earth System Science Data Discussions, 1-30.

Paulo E. Faria Junior, Koen A. de Mare, Klaus Zollner, Sigurdur I. Erlingsson, Mark van Schilfgaarde, Karel Vyborny, Sensitivity of the MnTe valence band to orientation of magnetic moments, [arXiv:2204.04206](https://arxiv.org/abs/2204.04206).

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

## Contributions to conferences

H. R. Heris, K. Klausen, A. Sitek, S. I. Erlingsson, A. Manolescu, Charge and heat currents in prismatic tubular nanowires, International Semiconductor Conference - CAS 2022, Romania, pp. 177-180, <https://doi.org/10.1109/CAS56377.2022.9934669> IEEE Xplore Digital Library (2022), [arXiv:2302.01742](https://arxiv.org/abs/2302.01742).

E. Fakhri, M. T. Sultan, A. Manolescu, S. Ingvarsson, H. G. Svavarsson, Germanium coated silicon nanowires as human respiratory sensing device, International Semiconductor Conference - CAS 2022, Romania, pp. 163-166, <https://doi.org/10.1109/CAS56377.2022.9934678> IEEE Xplore Digital Library (2022).

Kristján Klausen et al., “Andreev reflection and electron-hole coherence in proximitized core-shell semiconductor nanowires”, invited talk at the CMD29 conference in Manchester, 22 August.

Kristján Klausen et al., Electron-hole coherence in proximitized core-shell nanowires, Northern Lights Conference, Reykjavik 12-15 October.

K. Torfason, A. Valfells, A. Manolescu, Simulations of Thermionic Emission from Lab 6-Vb 2 Emitter, 2022 IEEE International Conference on Plasma Science (ICOPS), 22-26 May, IEEE *Xplore* DOI: [10.1109/ICOPS45751.2022.9813104](https://doi.org/10.1109/ICOPS45751.2022.9813104)

## Research plans for 2023

Phonon drag effect and heat conduction of nanowires, part of the PhD work of Hadi Rezaie.

Electrical characterization of respiratory sensors based on silicon 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 nanowires exposed to mechanical stress.

Simulations combined with machine learning of emission and propagation of electrons in vacuum microdiodes.