

Materials Science

M.Sc. education program

crei.skoltech.ru/cest/education/materials-science-program
msc.skoltech.ru/materials-science

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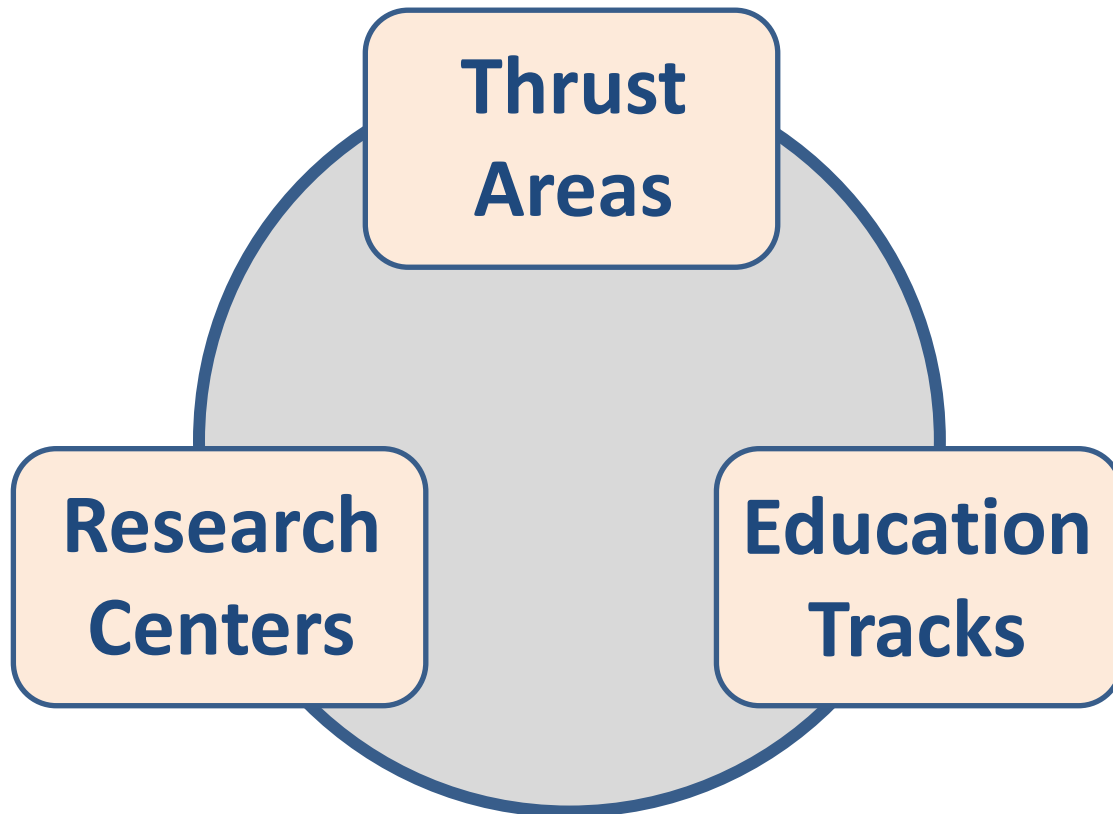
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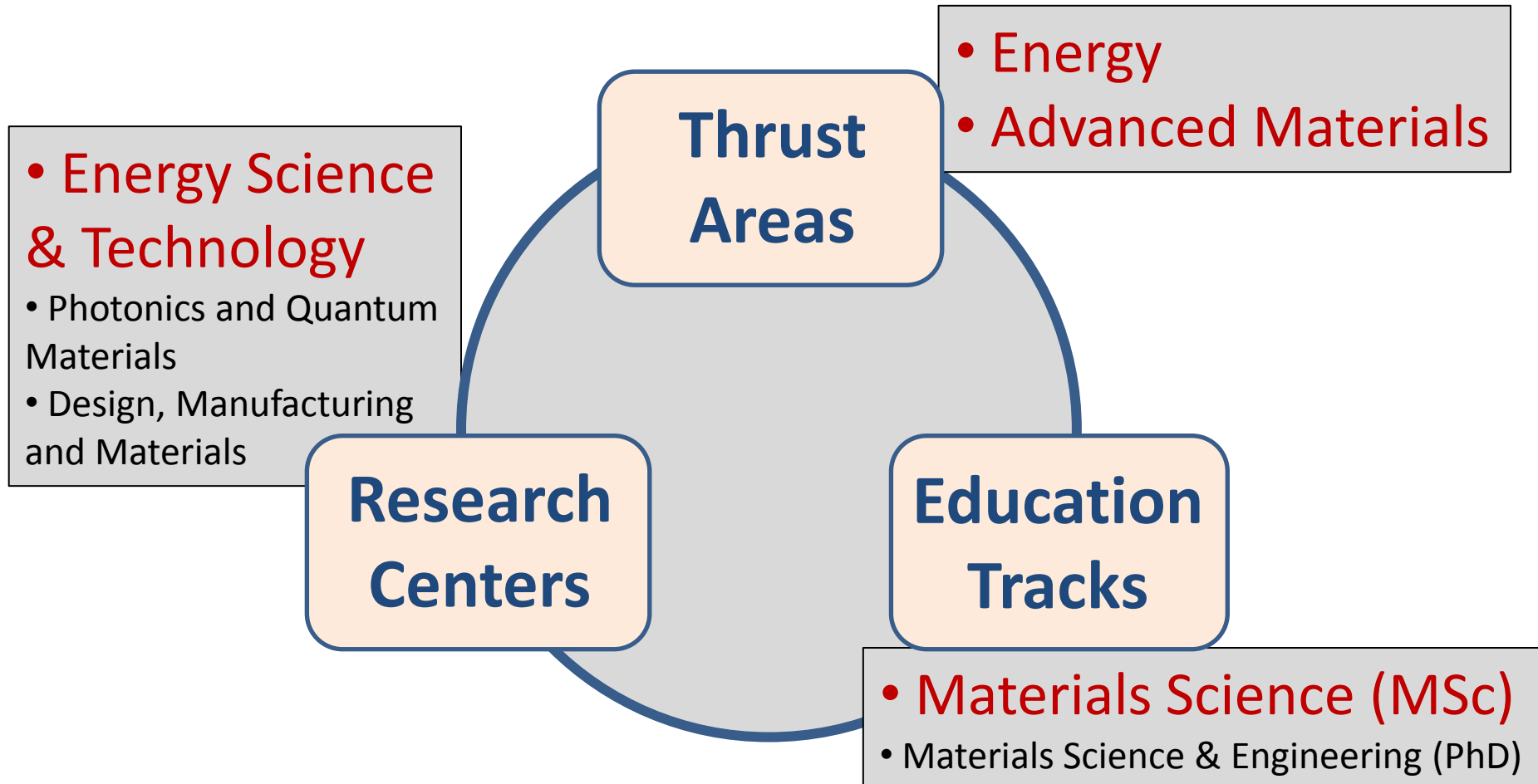
Skoltech research & education environment

- No separate theory or experiment departments
- No separate physics or chemistry departments



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What is (modern) Materials Science?

*Would not exist without
recent advances in
Materials Science*



Elementary devices/parts

- box/frame
- processor (transistors)
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- display
- battery
- thermal management
- wires, antennas, audio
- ...

Functional materials

- mechanical & chemical
- semiconductors
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Functional materials

- mechanical & chemical
- semiconductors
- light emitter
- battery electrodes
- thermal conductors
- thermal insulators
- ...

What do Materials Scientists do?

OLED vs LCD visualization



Above: Simulation of the difference in contrast from the AC7 OLED to a traditional LCD.

- Create new materials
- Optimize existing materials
- Create/study/optimize elementary devices (lab prototypes)

Materials Science track: courses

Core courses

- Survey of Materials (**Term 1B**)
- Materials Chemistry (**Term 2**)

Experimental Materials Science

Recommended courses

- Introduction to Solid State Physics(**2**)
- Material Structure Characterization Methods (**3**)
- Organic Materials for Electronics, Energy Conversion and Storage (**3**)
- Carbon Nanomaterials (**3**)
- Electrochemistry (**4**)

Computational Materials Science

Recommended courses

- Computational Chemistry and Materials Modeling (**2**)
- Structure and Property of Materials (**3**)
- Advanced Materials Modeling (**4**)
- Advanced Solid State Physics (**6**)
- Materials Selection in Design (**5**)

Elective courses

- discuss with your advisor

Career paths

Training time ↑

- (PhD+) **Research & teaching:**
 - Academic universities (e.g. Skoltech)
- (PhD) **Research:**
 - Universities (Skoltech, MIT)
 - Research institutions (Los Alamos Nat Lab)
 - R&D labs in large corporations (Samsung)
 - other high-tech companies
- (MSc) **Engineering, manufacturing, support etc.:**
 - Startups (batteries, solar cells, electronics)
 - Industry (energy, electronics, chemical)

Skoltech is the right place to start your career of a Materials Scientist or Engineer

Job market: Examples from high-tech industry

Advanced materials

- Boeing, Mitsubishi
- IMEC

Energy storage

- Tesla Motors
- Liotech

Energy conversion

- Heliatek, Solarmer

Electronics

- Samsung, IBM
- Plastic Logic

Chemical

- BASF, Chevron, DuPont

Automotive

- Nissan, KAMAZ

IT (materials modeling)

- Continuum Analytics, Gaussian, MedeA, Simbeyond
- Kintech (Skolkovo resident)

Skoltech will make you competitive on this market

RESEARCH DOMAIN

Changing the world through creative research

Future IT

Advanced Devices

New Materials

Research Paper

Research Infra

New Materials

Cutting-edge new materials is the critical factor of both the current as well future IT industries.

Research on new material enabling new display formats, such as reflective, transparent, and/or flexible displays and high-performance optical films and color-converting organics and inorganics are examples of activities necessary for such paradigm shifts.

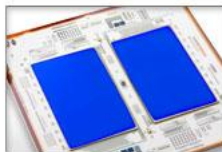
In addition to active electronics materials, SAIT is conducting research on new materials and processing technologies to foster High-performance yet environmentally friendly electronics technologies. Nanomaterial technologies offer an opportunity to reduce consumption of natural resources and energy in manufacturing as well as in the use of electronic devices.

Synthesis and incorporation into devices of graphene, quantum dots are examples of activities that SAIT is pursuing, based on our anticipation of a better future based on technology.

Organic Emitting Materials Flexible Electronics



OLED (Organic Light Emitting Diodes) is ... [More](#)



The advent of the so-called "ubiquitous ... [More](#)

Advanced Optical Film



Advanced optical film technology ... [More](#)

Functional Inorganics



Functional inorganics technology ... [More](#)

Nano Carbon Composite



Quantum Dot



Next-generation Battery



Energy Harvesting



Job market: Established partners for CEST CREI

- Multiple joint projects with MIT, MSU, MIPT

Joint Labs

- with MSU “Advanced Materials for Green Energy”
- with Institute of Problems of Chemical Physics
- with Mendeleev University

Academic – research and internships

- Los Alamos National Lab, University of Texas at Austin, Nanjing University, Johannes Kepler University

Academic – research

- University of Bayreuth (Volkswagen), University of Antwerp (research contract), University of Ulm (Helmholtz Institute), University at Albany (CRDF)
- EU framework project COST Action 1307 StableNextSol

Industry

- InEnergy, Systems for Microscopy and Analysis, Liotech, TAGRAS, KAMAZ
- LG, Bosch, Nissan, Samsung

Small companies

- SuperOx, Skolkovo startups

At Skoltech you will have access to partners via Research & Industrial “immersion”

Academic partners



**Massachusetts
Institute of Technology**



**Universiteit
Antwerpen**



A!
Aalto University



**COLLÈGE
DE FRANCE**
—1530—



N* Novosibirsk
State
University
*THE REAL SCIENCE



**TALLINN UNIVERSITY OF
TECHNOLOGY**



TUM
**TECHNISCHE
UNIVERSITÄT
MÜNCHEN**

Industrial partners



Startup company “K-plus” Ltd*



The goal of the project is a commercialization of promising electrochemical systems based on K-ion batteries. Develop technologies for cathode materials based on $K_xM[B(CN)_6]$ (where M, B are Fe, Co, Cr, Mn) cyanide transition metal complexes, and high-capacity carbon-based anode materials.

Startup company “Rustor” Ltd**



The main areas of work are cathode materials based on phosphates with the structure of olivine ($LiFePO_4$, $LiFe_{1-x}Mn_xPO_4$, also known as LFP and LFMP) and layered oxides ($LiNi_{1-x-y}Mn_xCo_yO_2$, also known as NMC).

Startup company “Core Technology”



Developed code USPEX allows to predict material crystal structure with arbitrary P-T conditions by knowing only chemical composition of the material. Company provides services to commercial companies in a field of prediction of structure and chemical composition of functionalized materials for different application.

Job market: Activities and events

Education-related activities

- 2-month Industrial Immersion
- 2-month Academic Mobility
- Industry Day

Research-related activities

- Research grants and Industrial contracts
- Scientific collaborations and visits

Entrepreneurship-related activities

- Startups (+support from E&I Center and Skolkovo Foundation)

Local events

- Skolkovo Innovation Center events
 - Startup Village, Open Innovations, Job and the City etc.
- Skoltech conferences (meet Industry and Academic representatives)
 - International School-Conference of Young Scientists (energy storage materials)
 - International School-Conference in Computational Materials Science
 - other Skoltech conferences in Materials Science and Engineering

At Skoltech you will have many opportunities to meet your future employer

M.Sc. Research in Materials Science

In brief

- *Highly interdisciplinary*
- Materials for energy storage – Abakumov, Antipov, Stevenson
- Optoelectronic materials – Nasibulin, Troshin
- Structural materials – Korsunsky
- Computational Materials Science – Gonze, Levchenko, Oganov, Shapeev, Tretiak, Zhugayevych
- Theoretical Materials Science – Buchachenko, Fine
- ... *with details on faculty web-pages: [example](#)*

M.Sc. Thesis 2016-2019

- Materials for energy conversion and storage (19 students)
- Materials for optoelectronics (8 students)
- Computational materials science (4 students)
- Other materials (2 students)

At Skoltech you will do world-level research at cutting edge of science

Broad range of topics: see e.g. public media reports



4/12/2019

Skoltech PhD student, Roman Kapaev, on potassium batteries. [Watch on Rossiya 1](#)



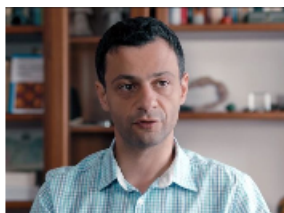
28/11/2019

Albert Nasibulin and his colleagues have created a transparent film based on nanotubes. [Read on Izvestia](#), [popmech.ru](#)



11/11/2019

A group of scientists led by Pavel Troshin have developed superfast charging high-capacity potassium batteries based on organic. Read on [EurekAlert!](#), [Indicator](#), [Poisknews](#), [popmech](#), [phys.org](#), [newinform](#), [openscience.news](#), [bitcryptonews](#), [pv-magazine](#), [azom.com](#)



7/11/2019

A group of scientists led by Artem Oganov have succeeded in synthesizing thorium decahydride (ThH₁₀), a new superconducting material with a very high critical temperature (161 K). Read on [TASS](#), [Naked Science](#), [Interfax](#), [Indicator](#), [Regnum](#), [N+1](#), [Yandex.news](#), [news.sputnik.ru](#), [sib-science.info](#), [rscf.ru](#), [scitechdaily.com](#), [techsite.io](#), [nanotech-now.com](#), [Phys.org](#), [chemeurope.com](#)



31/10/2019

Skoltech Ph.D. student, Olga Kraevaya and her colleagues from the Institute for Problems of Chemical Physics of Russian Academy of Sciences and National Taiwan University have discovered that fullerene compounds can help in the fight against lung cancer. Read on [TASS](#), [EurekAlert!](#), [NakedScience](#), [popmech.ru](#), [meddaily.ru](#)



23/08/2019

Alexei Salimon and his colleagues from IPAC RAS and MISIS developed a new technology for producing ultra-high molecular weight polyethylene with a porous structure. Read on [TASS](#), [Rambler.news](#), [Indicator](#), [Gazeta.ru](#), [mk.ru](#), [news.Sputnik](#), [nauka.vesti.ru](#)



7/08/2019

Alexander Kvashnin and his colleagues presented the research optimizing the search for new materials that can replace diamonds in drilling rigs. Read on [Phys.org](#), [Nauchnaya Rossiya](#), [Vechernyaya Moskva](#), [RIANovosti](#), [Chrdk](#), [goroday.ru](#), [bitcryptonews.ru](#)



3/06/2019

Skoltech scientists have created a new polymer cathode material for fast-charged metal-ion batteries that surpasses all previous similar developments. [Read on Naked Science](#), [RIANovosti](#), [Indicator](#)



26/05/2019

Skoltech scientists and their American colleagues have created artificial intelligence, accelerating quantum calculations. Read on [RIANovosti](#), [scientificrussia.ru](#)

Laboratories in Materials Science

Experiment (*visit Lab Tours*)

- Multifunctional [Energy Storage Lab](#)
- [Laboratory of Nanomaterials](#) (Nasibulin)
- other [CEST CREI facilities](#)
- partners (MSU, MIPT, IPCP, Mendeleev U)

Theory (software+hardware)

- Multifunctional [Computational Materials Science Lab](#)
- [USPEX Lab](#) (Oganov, computational materials discovery)
- partners (MSU, LANL)

Skoltech shared facilities

- [Advanced Imaging Core Facility](#)
- [FabLab and Machine Shop Shared Facility](#)

At Skoltech you will have access to unique facilities

Computational Materials Science Laboratory (CMS Lab)

Our CREI has comprehensive toolset and expertise for modeling of organic and inorganic materials from large scale classical molecular dynamics to highly accurate ab initio quantum chemistry. Core facilities are consolidated as **CMS Lab**, whereas two other labs provide unique specialized tools: [structure prediction](#) (Artem R. Oganov) and [machine-learning interatomic potentials](#) (Alexander Shapeev).

Expertise in materials modeling

- [Dmitry Aksenov](#) – inorganic materials for energy storage
- [Xavier Gonze](#) – inorganic semiconductors for various applications
- [Sergey Levchenko](#) – catalysts
- [Sergei Tretiak](#) – organic and perovskite semiconductors for optoelectronics
- [Andriy Zhugayevych](#) – organic semiconductors for various applications

Hardware

- 224-core CEST CREI cluster Magnus highly optimized for DFT-level materials modeling
- [Access to 628-core Skoltech cluster Pardus](#)
- [Access to 2048-core CDISE cluster Arkuda](#)
- CEST CREI storage and exchange miniserver
- 2 terminals for MSc students

Software and primary technical experts

- [LAMMPS](#) (classical molecular dynamics) – Andriy Zhugayevych
- [MOPAC](#) (semiempirical methods) – Andriy Zhugayevych
- [VASP](#) (quantum chemistry of solids) – Dmitry Aksenov
- [Gaussian](#) (quantum chemistry of molecular systems) – Nikita Tukachev
- [Molpro](#) (quantum chemistry of molecules) – Nikita Tukachev, Dmitry Bezrukov
- [FHI-aims](#) (quantum chemistry with numerical atomic orbitals) – Sergey Levchenko
- [Abinit](#) (quantum chemistry of solids) – Xavier Gonze
- [NEXMD](#) (nonadiabatic excited-state molecular dynamics) – Sergei Tretiak

No other regional lab in CMS has such a broad expertise & set of tools

What is special about Materials Science at Skoltech?

1) Broad coverage of topics

- 12 special courses + >10 topical electives
- Several state of the art Labs

2) Distinguished faculty – median h-index > 35

- Cutting edge of science
- Great presenters

3) General Skoltech excellence

- Broad selection of elective courses
- Support of Entrepreneurship and Innovation
- Industrial immersion and Academic mobility
- Modern education – interactive learning

Welcome to Skoltech

Further information:

- Lab Tour
- crei.skoltech.ru/cest/education/materials-science-program
- msc.skoltech.ru/materials-science
- If you are interested to join a specific research project contact our faculty