Survey of Materials

Introduction

Andriy Zhugayevych

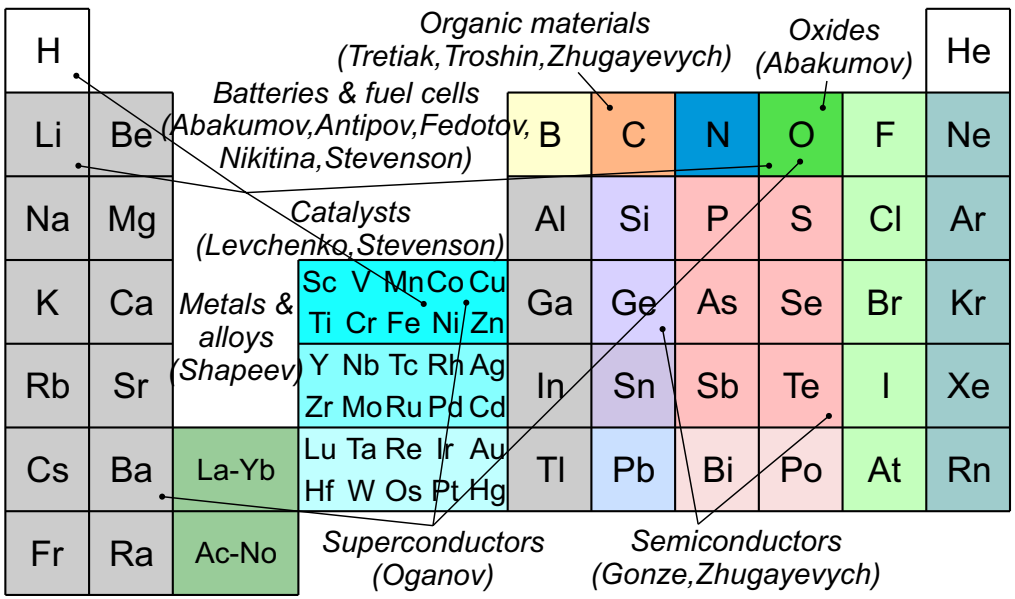
September 30, 2021

Outline

- What is this course about
- Case study 1: solar cells – energy generation
- Case study 2,3: batteries – energy storage
- Part II overview
- Course logistics

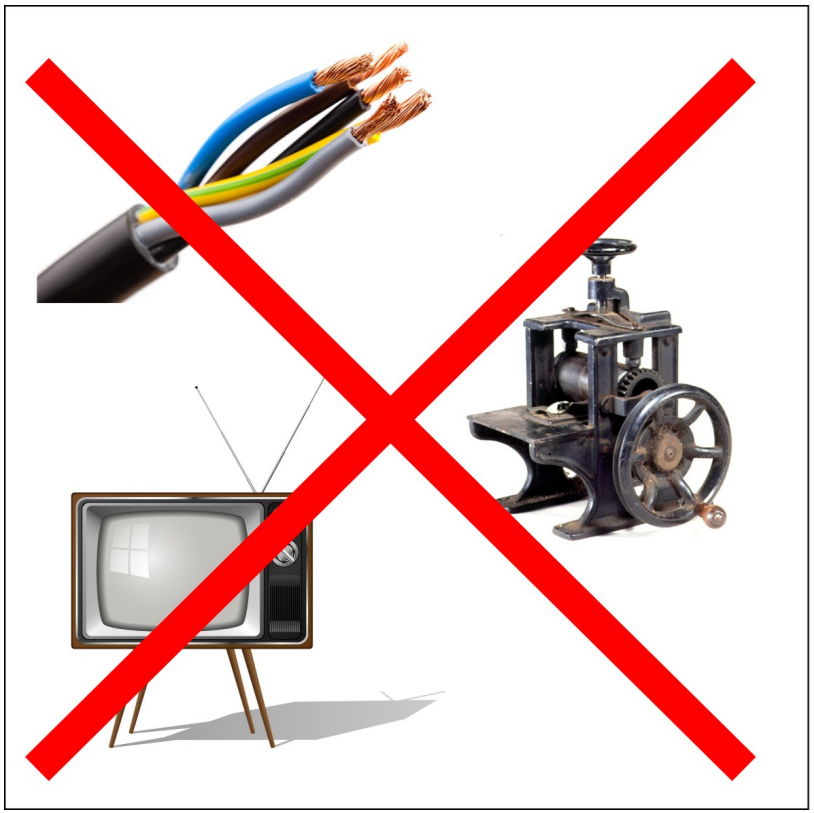
What is this course about

- Part I (1 week): Four classes on fundamentals of Materials Science
- Part II (2 weeks): Material-centered introduction to Materials Science given by experts in the corresponding field



Also: Perovskites for optoelectronics (Tretiak,Troshin), Carbon nanomaterials (Nasibulin), Materials at high-pressure (Oganov), Hierarchically structured materials (Korsunksy)

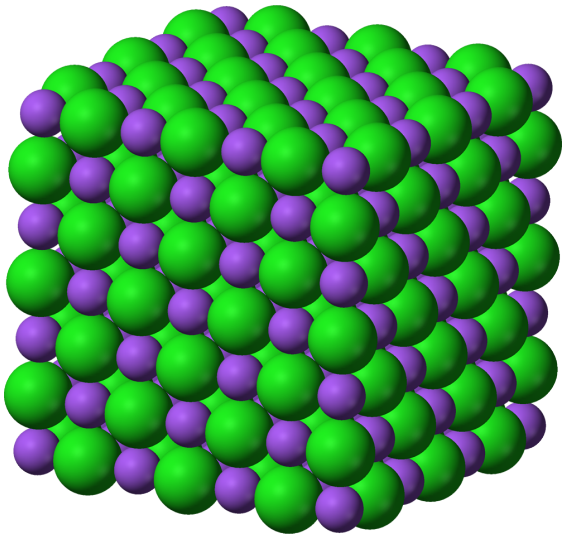
What materials are covered



- New materials or new technologies
- Under research at Skoltech

What scales are covered

microscale



just a NaCl

macroscale

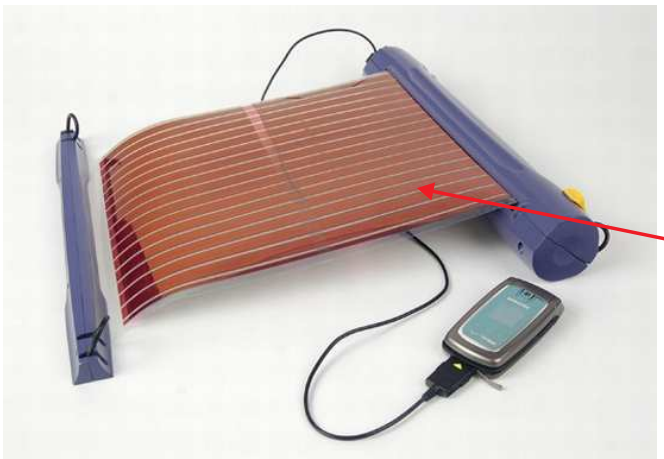
×many 'flavors'

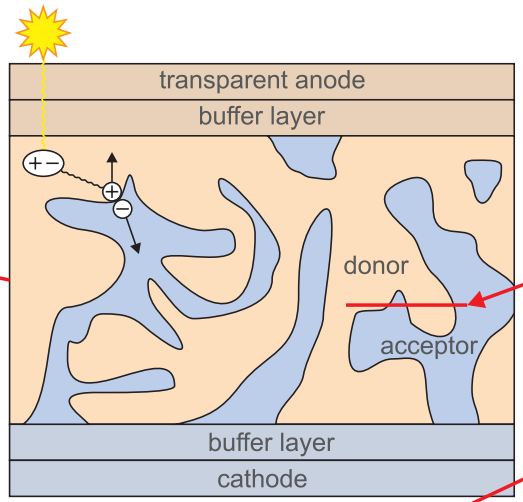
device scale

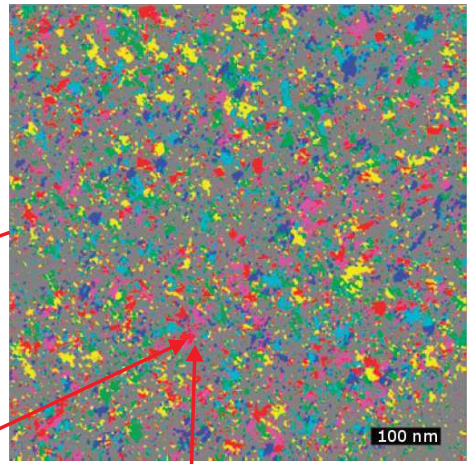
×many applications

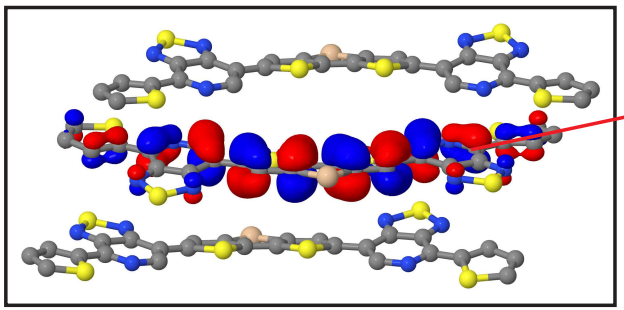
- Materials Science starting from microscopic scale and up to what can be covered in a single lecture

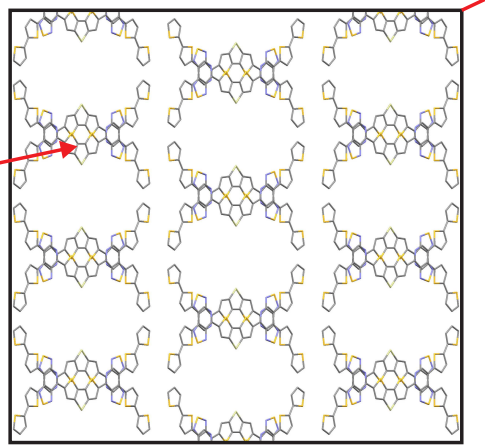
What scales are covered (more complex example)

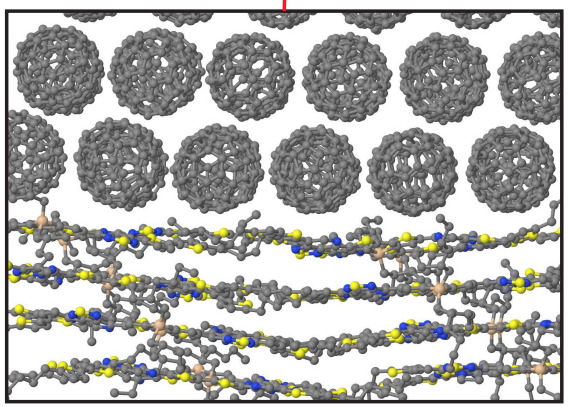












Level of coverage

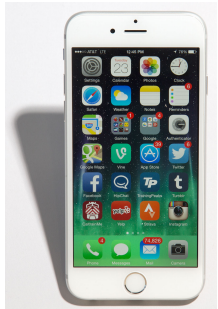
Basics + Overview + Readiness to special courses in Materials Science:

- *General courses*
  - Materials Chemistry
  - Materials Physics (Introduction to Solid State Physics)
  - Materials Engineering (Applied Materials and Design)
- *Modeling*
  - Materials Modeling (& Computational Chemistry + Advanced)
  - Structure and Property of Materials
- *Characterization*
  - Materials Structure Characterization
  - Electrochemistry
- *Specific materials*
  - (Materials for Energy Storage and Conversion)
  - Organic Materials
  - Carbon Nanomaterials

See roadmap here:

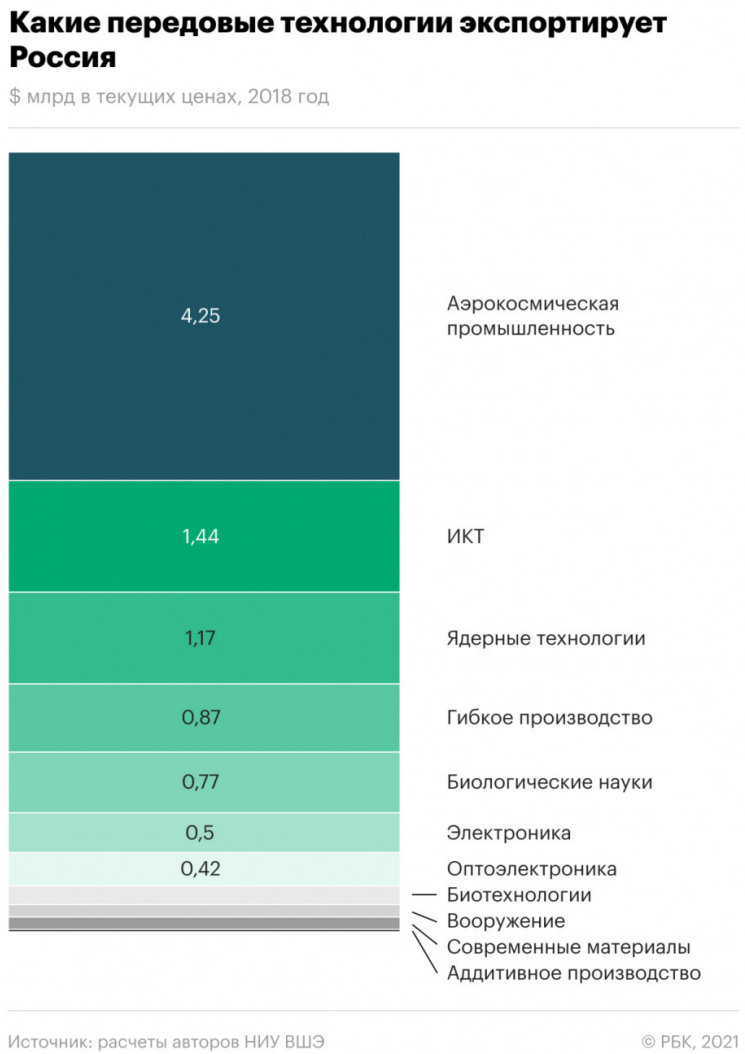
crei.skoltech.ru/cest/education/materials-science-program

Addressing regional challenges in high-tech manufacturing



Where is the bottleneck?

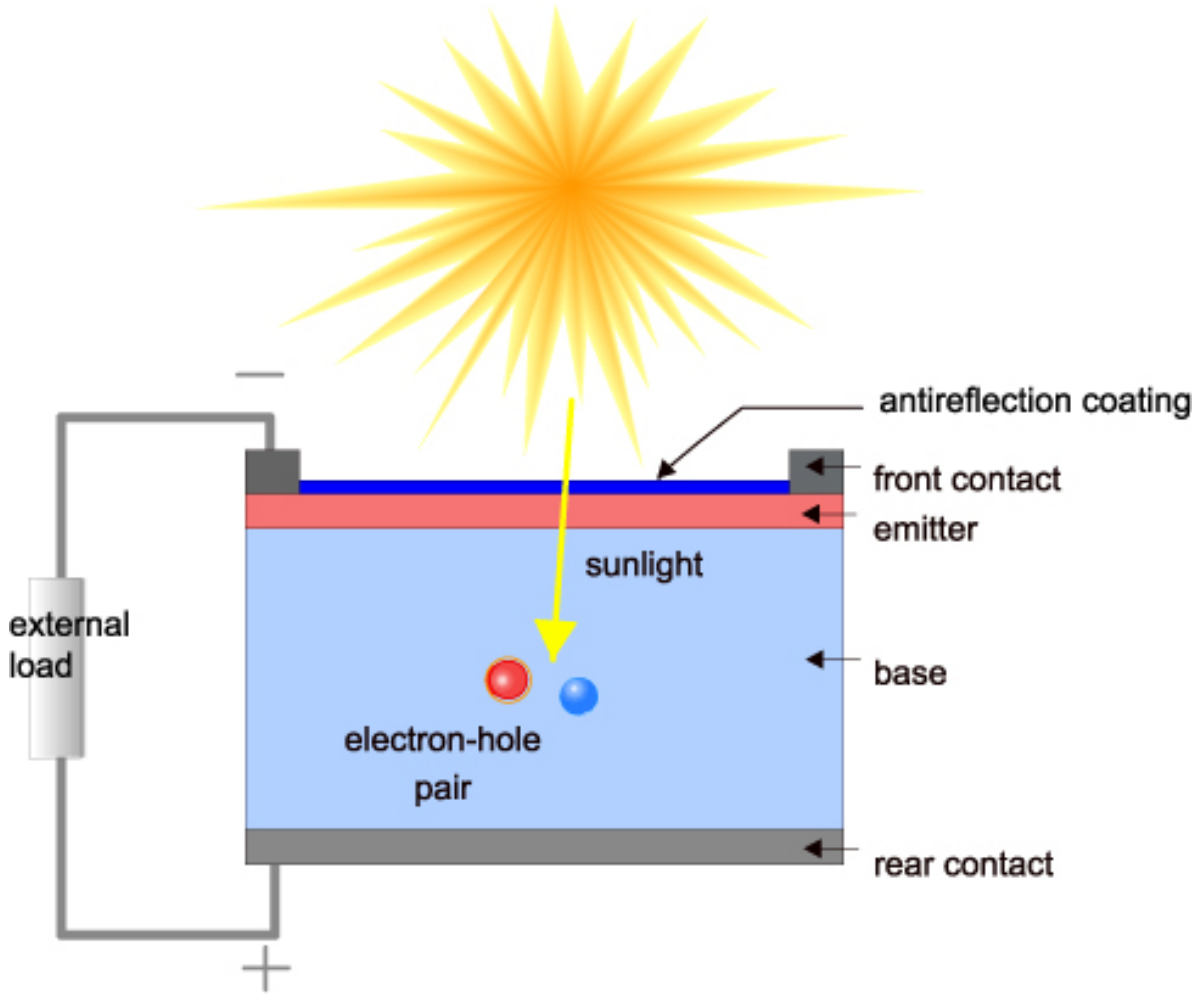
- feedstock
- materials
- parts
- assembly
- software
- sales
- service



Materials Science & Engineering addresses materials + parts

Case study 1: Solar cells

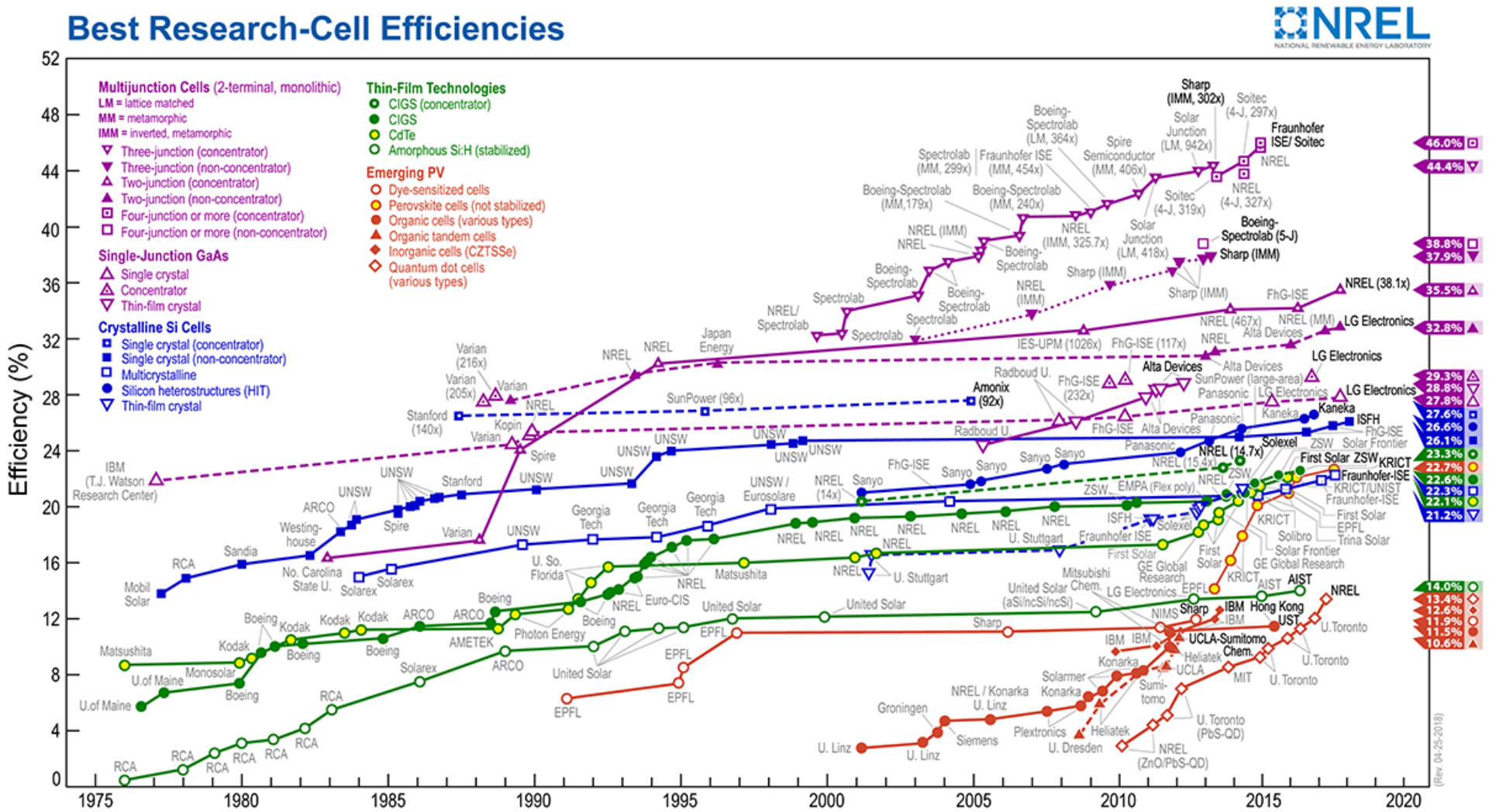
CEST CREI Research Thrust



www.pveducation.org

Understand $\rightarrow$ Optimize $\rightarrow$ Design $\rightarrow$ Manufacture

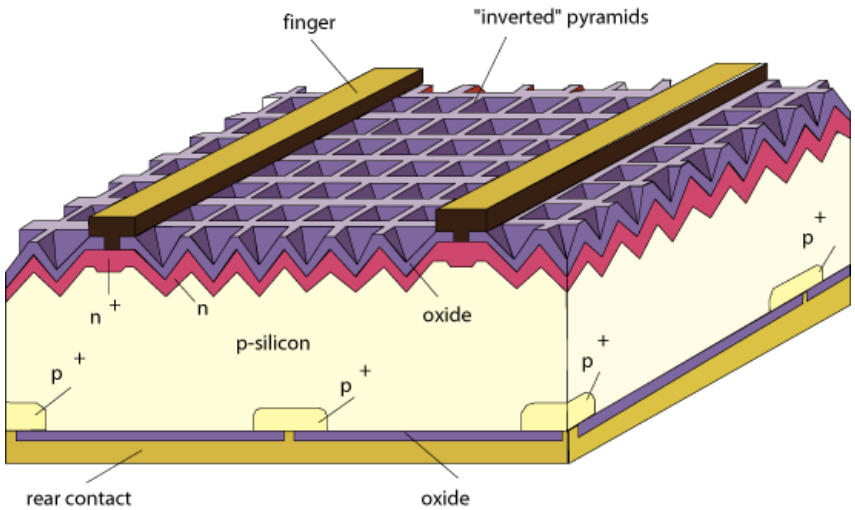
Power conversion efficiency

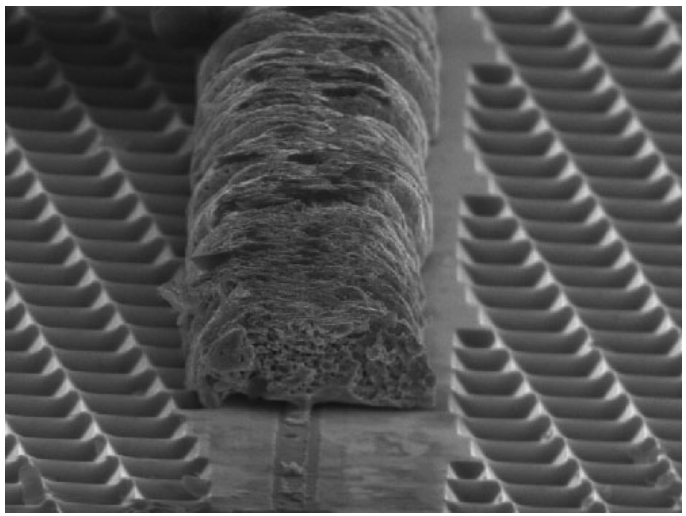


Reference: NREL chart

75-year evolution of Si solar cells: from 0 to 25%

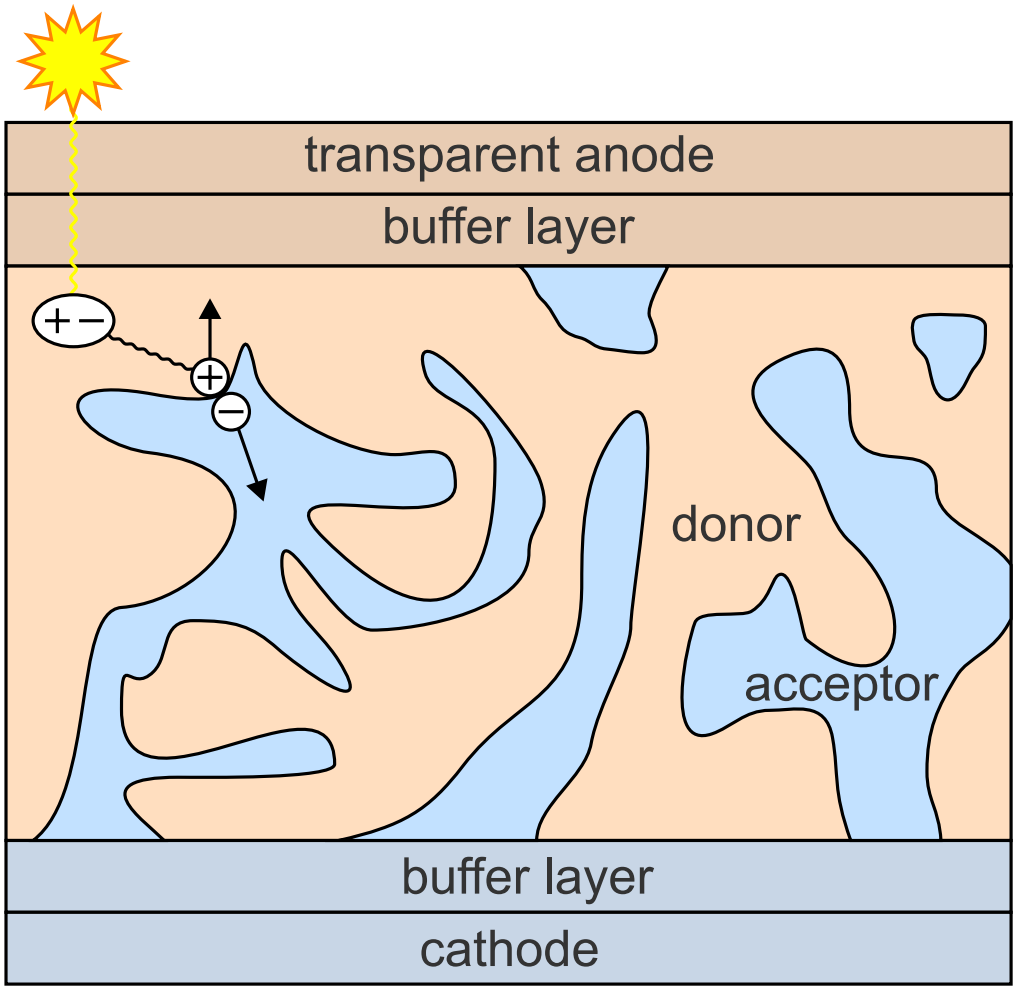
PERL – passivated emitter with rear locally diffused cell:





Reference: pveducation.org

Bulk-heterojunction solar cells (from 0 to 18% in 20 years)



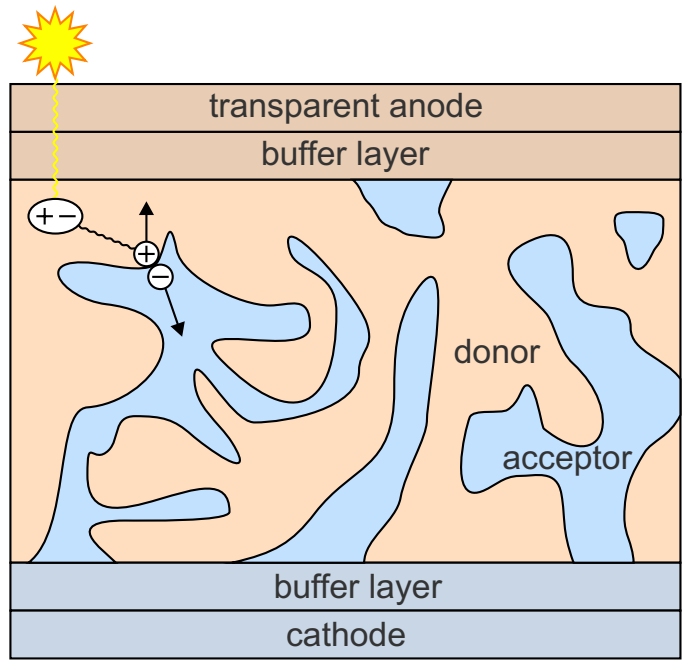
Optimize performance:

- Donor material
- Acceptor material
- Interface
- Morphology
- Contacts
- Light absorption
- Aging
- ...

$\Longrightarrow$ Structure & properties: 1) bulk material, 2) surface/interface

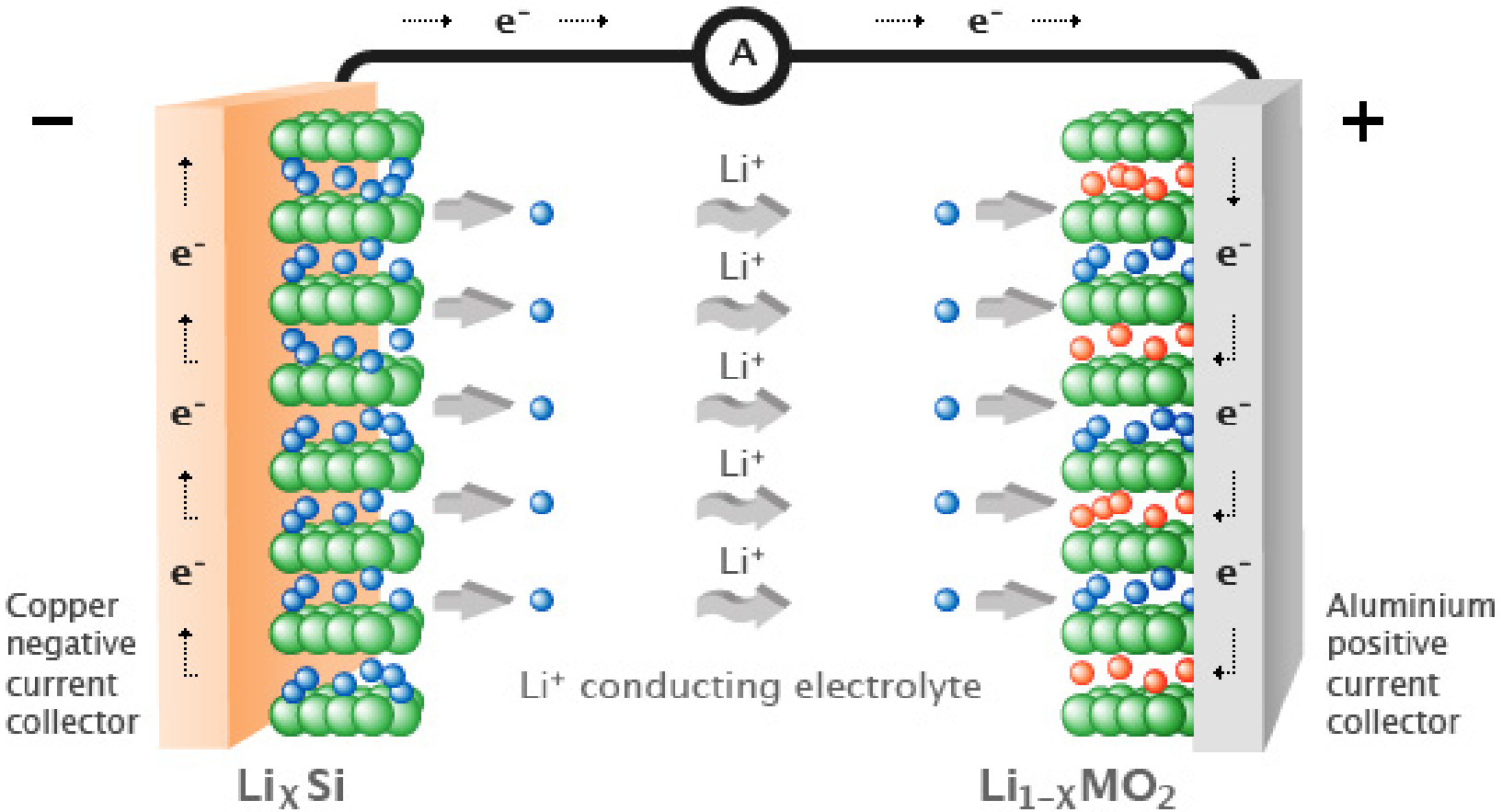
Properties to study and optimize

- Sunlight harvesting efficiency
- Exciton diffusion length
- Energy of charge carriers
- Mobility of charge carriers
- Efficiency of charge separation
- Degradation and aging



Case study 2: Metal-ion batteries

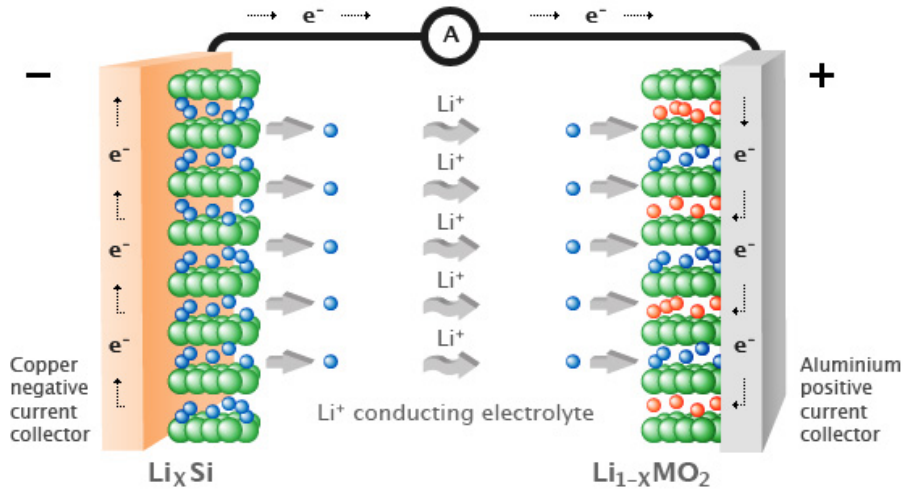
CEST CREI Research Thrust: two startup companies created – "Rustor" and "K-plus"



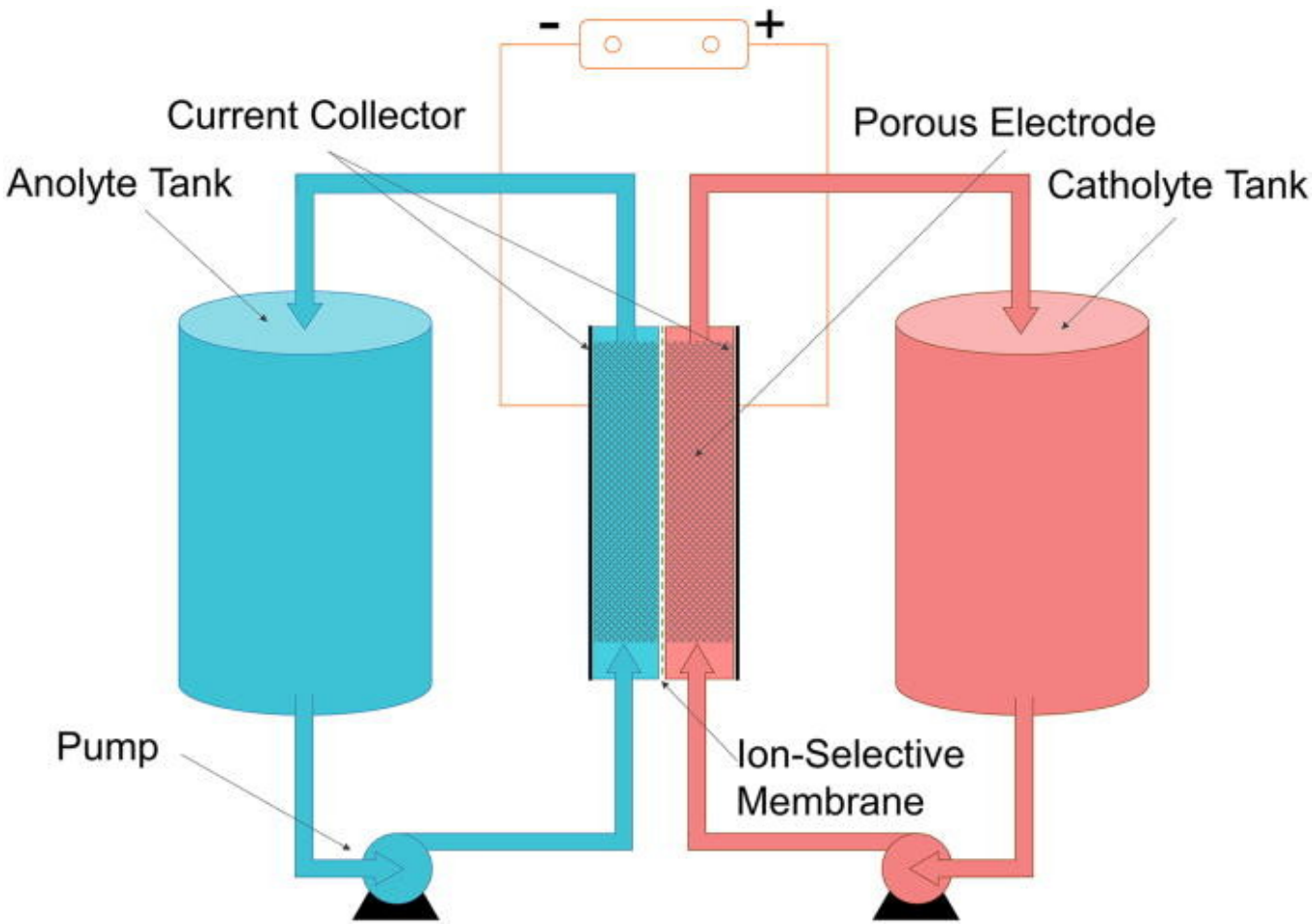
nexeon.co.uk

Properties to study and optimize

- Energy of charge carriers
- Diffusivity of charge carriers
- Cathode/anode capacity
- Charge/discharge reversibility
- Degradation and aging

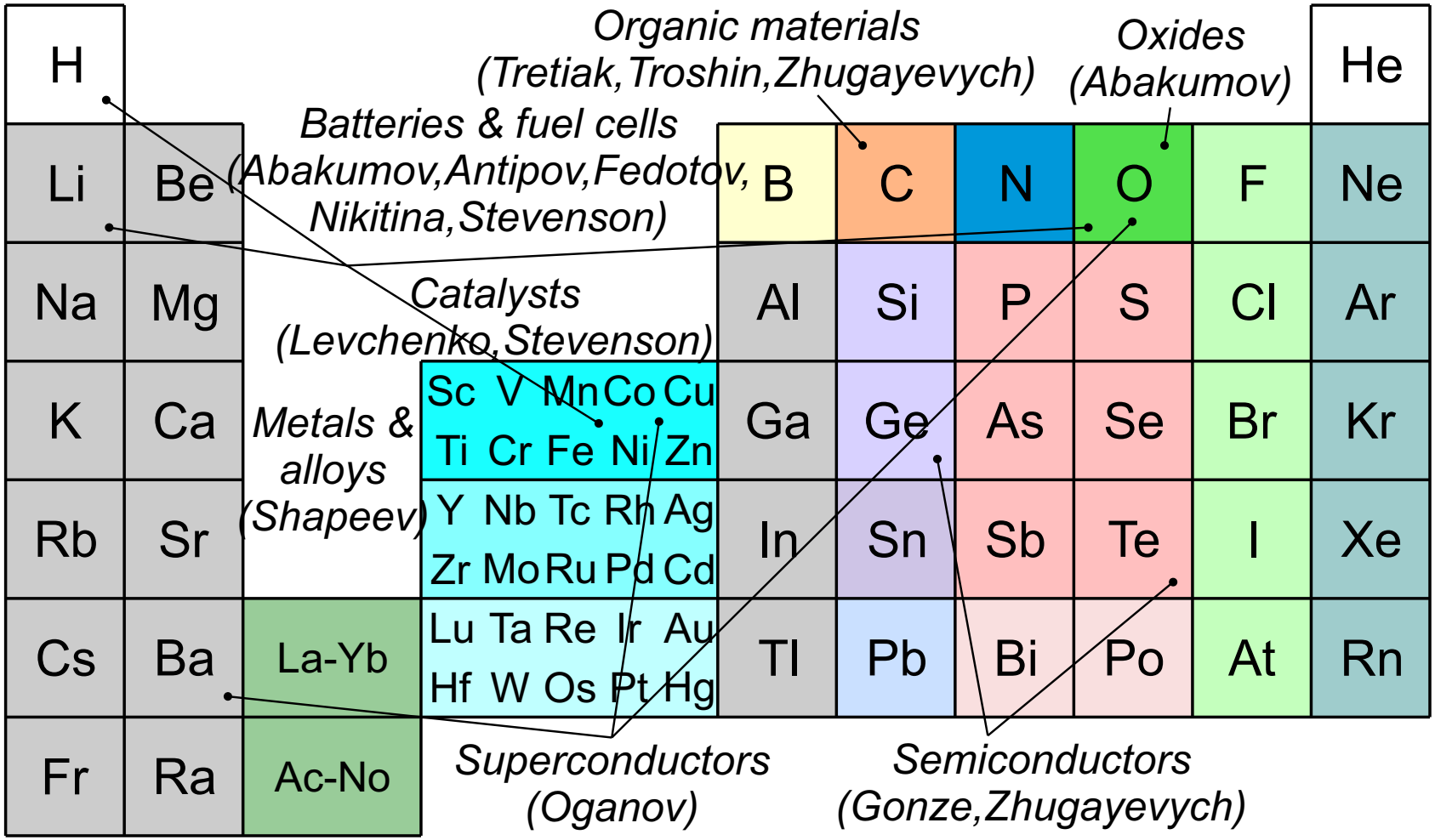


Case study 3: Redox flow batteries



The same concept but different device architecture $\Longrightarrow$ different materials needed, different structure-property relationships

Part II overview: chemical composition perspective



Also: Perovskites for optoelectronics (Tretiak,Troshin), Carbon nanomaterials (Nasibulin), Materials at high-pressure (Oganov), Hierarchically structured materials (Korsunksy)

Part II overview: applications perspective at Skoltech

- Materials for energy generation, conversion, storage: CEST CREI, *Abakumov, Antipov, Fedotov, Levchenko, Nikitina, Stevenson, Tretiak, Zhugayevych*
- Optoelectronic materials: *Gonze, Gorin, Levchenko, Nasibulin, Tretiak, Zhugayevych*, CPQM CREI
- Composites: CDMM CREI
- Hydrocarbons: CHR CREI
- High-T superconductors: *Oganov*
- Metals and alloys modeling: *Shapeev*
- Materials nano-engineering: *Korsunksy*

Course logistics

- Course web-page
- Syllabus
- Schedule and timeline
- Required software
- Part I exam: theory and practice
- 40 hours per week:
  - 12 in class
  - 13 reading and self-study (!)
  - 15 homeworks and projects
  - see details here
- In-class mode with online exceptions

Bookmark these pages: Schedule, Canvas-2021, Course web-page

Learning outcomes explained

See Syllabus for complete list

- Level your background (not to replace background courses)
- Introduce Materials Science language and concepts
  (be able to understand Materials Science papers and talks)
- Be familiar with Materials Science research at Skoltech
- Know classes of materials studied at Skoltech
- Know state of the art in a specific research area
- Expand your set of practical skills in Materials Science
  (no labs or hands-on experience in this course)
- Here you can find or start research project (literature review)

Homework

- Familiarize yourself with course website
- Read carefully Syllabus
- Select at least one textbook for home reading
- Install required software
- Read and follow Skoltech policy on Academic Integrity
  (you will not pass this course without following those rules)
- Read and follow COVID safety guidelines