Survey of Materials

Introduction

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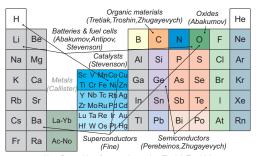
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Outline

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

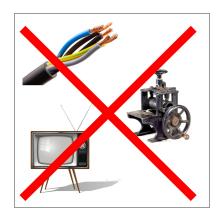
What is this course about

- Part I (1 week): Fundamentals of Materials Science to be able to understand Part II
- Part II (2 weeks): A set of independent lectures about materials 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



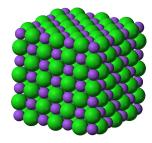


- New materials or new technologies
- Under research at Skoltech

What scales are covered

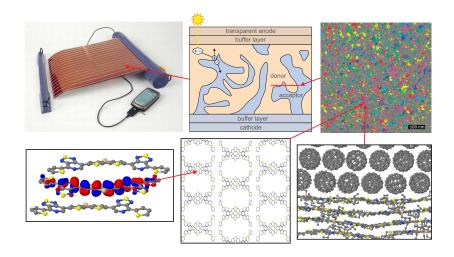






- Materials Science starting from microscopic scale
- Don't forget about other scales (meso-, macro-, device) and Materials Engineering and Technology

What scales are covered



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 (Materials Selection in Design)
- Modeling
 - Materials Modeling (& Computational Chemistry + Advanced)
 - Advanced Solid State Physics
 - Structure and Property of Materials
- Characterization
 - Materials Structure Characterization
 - Electrochemistry
- Specific materials
 - ► (Electrochemical Energy Storage Materials)
 - Organic Materials
 - Carbon Nanomaterials

See roadmap here:

Addressing regional challenges in high-tech manufacturing

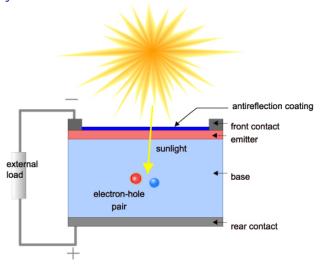


Where is the bottleneck?

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

MSE addresses materials + parts

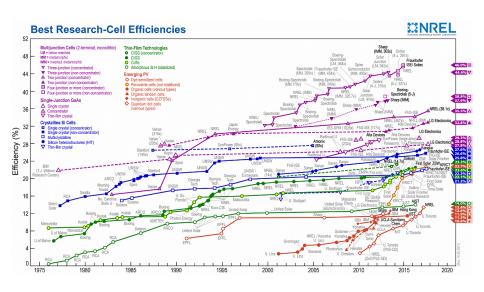
Case study 1: Solar cells



www.pveducation.org

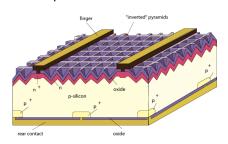
 $\mathsf{Understand} \to \mathsf{Optimize} \to \mathsf{Design} \to \mathsf{Manufacture}$

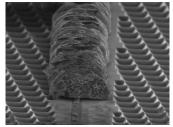
Power conversion efficiency



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

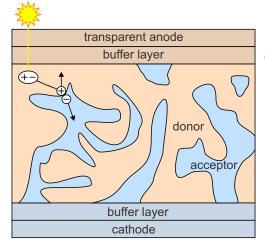
PERL – passivated emitter with rear locally diffused cell:





Reference: pveducation.org

Bulk-heterojunction solar cells



Optimize performance:

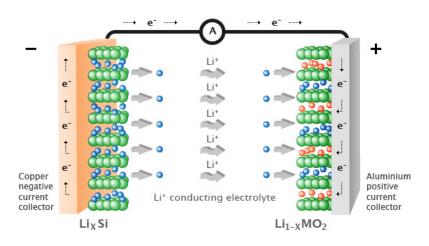
- Donor material
- Acceptor material
- Interface
- Morphology
- Contacts
- Light absorption
- Aging
- . . .

 \implies 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: Li-ion batteries



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

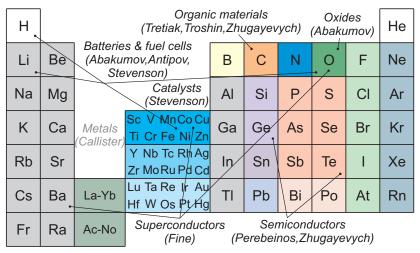
Course logistics

- Course web-page
- Syllabus
- Schedule and timeline
- Required software
- Part I exam: theory
- 40 hours per week:
 - ▶ 12 in class
 - ▶ 10-20 homeworks and projects
 - ▶ 10-20 reading and self-study

Part II overview: learning outcomes

- Level your background (not to replace background courses)
- Be able to understand Materials Science papers and talks
- Learn about a class of materials
- Know state of the art in a specific research area
- Be familiar with Materials Science research at Skoltech
- Here you can find or start research project

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

- Energy conversion and storage (CEST CREI):
 materials for energy generation, conversion, storage
 Abakumov, Antipov, Korsunksy, Oganov, Stevenson, Tretiak,
 Troshin, Zhugayevych
- Photonics and quantum materials (CPQM CREI):
 materials for electronics, spintronics, photonics
 Fine, Nasibulin, Perebeinos
- Design, manufacturing and materials (CDMM CREI): composites
- Hydrocarbon recovery (CHR CREI): hydrocarbons
- Space CREI: materials and devices
- Life Sciences CREI: devices, "biomatter", drugs