Survey of Materials

Introduction

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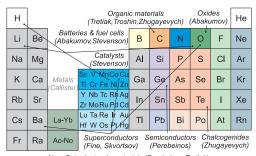
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Outline

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

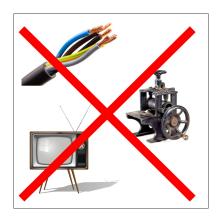
What is this course about

- Part I (4 lectures): Fundamentals of Materials Science to be able to understand Part II
- Part II (6 lectures): A set of independent lectures about materials given by experts in the corresponding field



Also: Optoelectronic materials (Perebeinos, Tretiak), Carbon nanomaterials (Nasibulin), Materials at high-pressure (Oganov)

What materials are covered



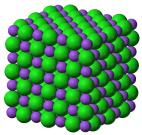


- New materials or new technologies
- Under research at Skoltech

What scales are covered

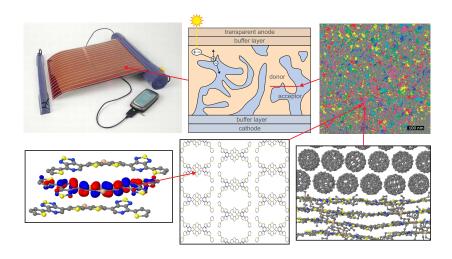






- Materials Science starting from microscopic scale
- Don't forget about other scales (meso-, macro-, device) and Materials Engineering and Technology

What scales are covered



Level of coverage

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

- General courses
 - Materials Chemistry
 - Materials Physics (Intro Solid State Physics)
- Modeling
 - Materials Modeling (and Computational Chemistry)
 - Device Modeling (Fundamentals of Device Physics)
 - Solid State Physics (Advanced)
 - Structure and Property of Materials
- Characterization
 - Materials Structure Characterization
 - Electrochemistry
- Specific materials
 - Organic Materials
 - Carbon Nanomaterials

See roadmap here: crei.skoltech.ru/cee/education

Addressing regional challenges

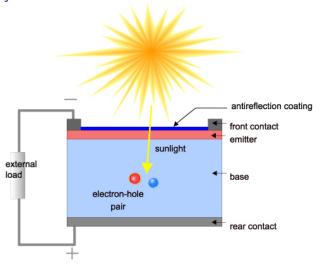


Where is the bottleneck?

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

MSE addresses materials + parts

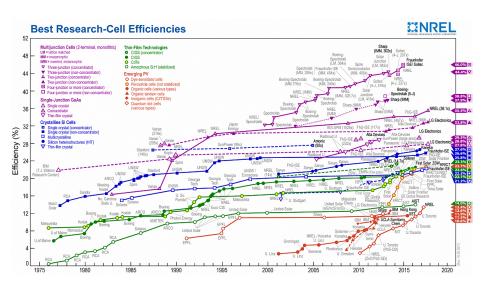
Case study 1: Solar cells



www.pveducation.org

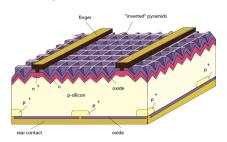
 $\mathsf{Understand} \to \mathsf{Optimize} \to \mathsf{Design} \to \mathsf{Manufacture}$

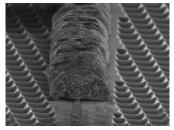
Power conversion efficiency



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

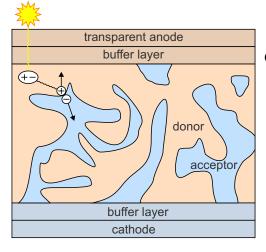
PERL – passivated emitter with rear locally diffused cell:





Reference: pveducation.org

Bulk-heterojunction solar cells



Optimize performance:

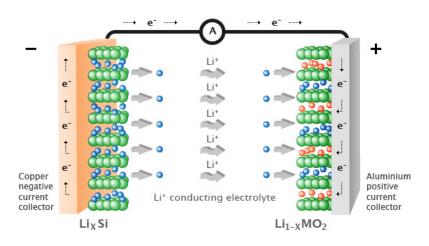
- Donor material
- Acceptor material
- Interface
- Morphology
- Contacts
- Light absorption
- Aging
- ...

⇒ 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

H	Organic materials Oxides (Tretiak,Troshin,Zhugayevych) (Abakumov)								Не
Li	Be	Batter (Abaku	В	C	N	0	F	Ne	
Na	Mg		Catalysts (Stevenson)	Al	Si	P/	S	CI	Ar
K	Ca	Metals (Callister)	Sc V MnCoCu Ti Cr Fe Ni∫Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	(Gameter)	Y Nb Tc Rh Ag Zr MoRu Pd Cd	I In∕	Sn	Sb	Te,	ı	Xe
Cs	Ba	La-Yb	Lu Ta Re Ir Au Hf W Os Pt Hg	TI	Pb	Bi	Ро	At	Rn
Fr	Ra	Ra Ac-No Superconductors Semiconductors Chalcogenides (Fine, Skvortsov) (Perebeinos) (Zhugayevych)							

Also: Optoelectronic materials (Perebeinos,Tretiak), Carbon nanomaterials (Nasibulin), Materials at high-pressure (Oganov)

Part II overview: applications perspective at Skoltech

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