Organic Materials for Energy and Optoelectronics

Course Introduction and Logistics

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Outline

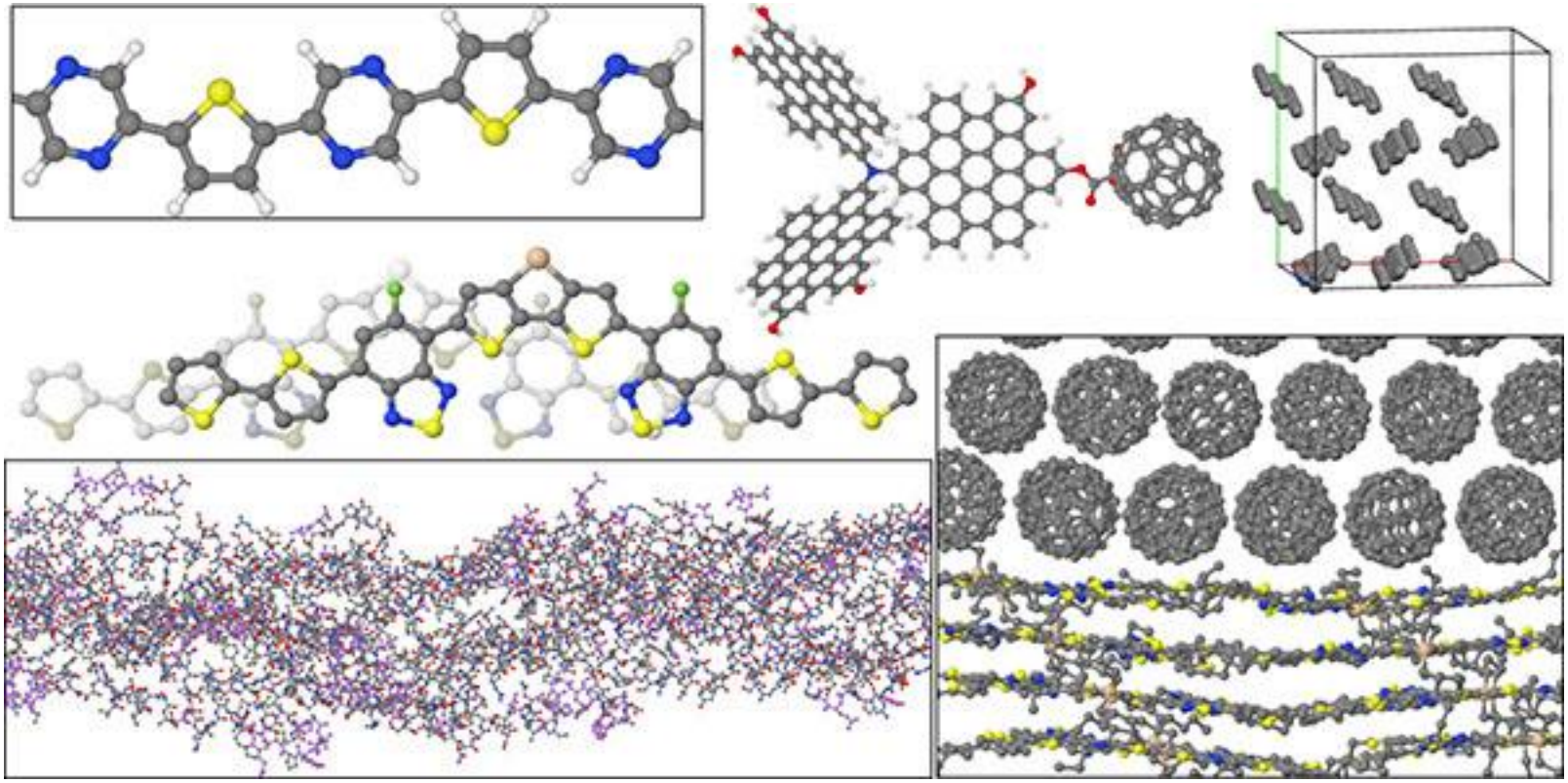
- What is this course about
- Relation to Skoltech education and research programs
- Course logistics

What is this course about

This course is about…

(1) organic materials…

(2) for energy and optoelectronics



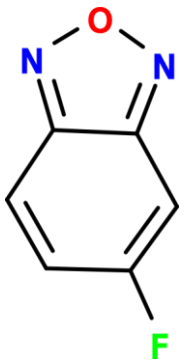
What is organic material

- *Generally speaking:*

Organic material is any carbon-based material except for CO, CO2, CN, carbides, carbonates etc

- *More rigorous definition is possible:*

Any material isostructural and isoelectronic to CH-only structure

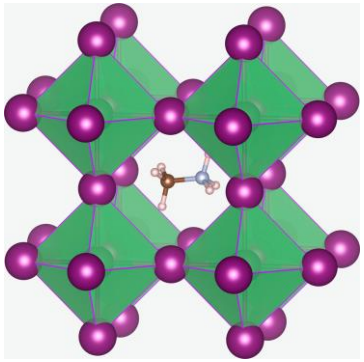


→ Replace
F by H or CH3,
O by CH2,
N by CH

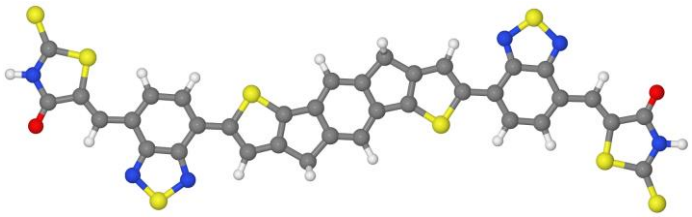
Organic vs inorganic

- Tiny fraction of chemical elements (mainly C, H, N, O) but immense variety of structural forms:
  - ICSD has 250 000 crystals
  - vs CSD with >1M crystals
  - and organics is usually non-crystalline

- Different approaches are used for organic and inorganic materials. Discuss example of perovskite solar cells



Classes of organic matter

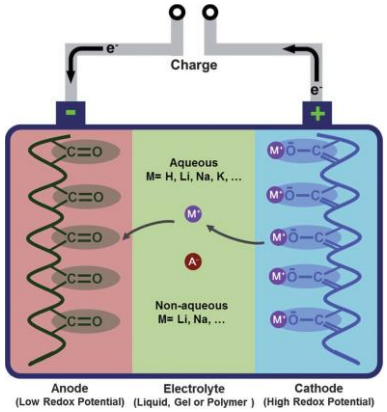


- Organic semiconductors (π-conjugated)
  – subject of this course
- Simple hydrocarbons (oil and gas industry)
  – but upon aging they loose hydrogens becoming π-conjugated
- Biological matter
  – but there are many π-conjugated fragments playing important role in biological processes (light harvesting, vision)
- Other electronically inactive organic materials such as non-semiconducting polymers and medical drugs
  – but many of them are π-conjugated, e.g. kevlar
- Hybrid organic-inorganic, e.g. metal-organic or hybrid perovskites – some of them will be considered in this course

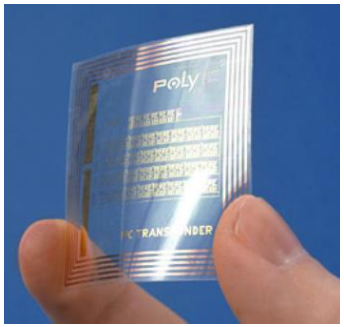
Applications in focus of this course

- Solar cells

- Rechargeable batteries



- Field effect transistors



- Light emitters

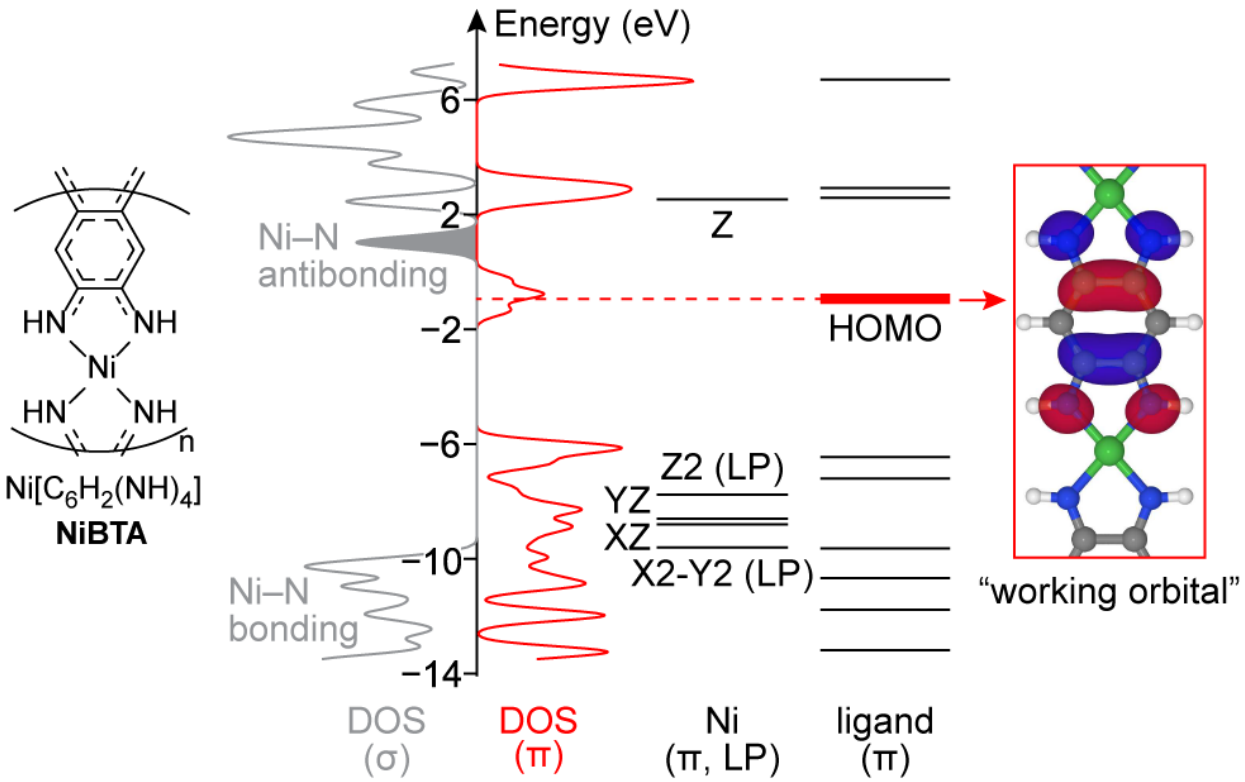
Organic materials studied at Skoltech

- For rechargeable batteries (CEST CREI, Keith Stevenson)
  - cathode or anode in metal-ion batteries
  - catholyte or anolyte in redox flow batteries
  - pure carbon as anode and conductive additive
  - polymer additives
- For solar cells (CEST CREI, currently inactive, Pavel Troshin)
  - active layer
  - charge transport layer for perovskite solar cells
- Carbon nanotubes (Albert Nasibulin)
  - sensors
- Theoretical studies (CEST CREI, Sergei Tretiak, Andriy Zhugayevych)
- Fragmentary studies
  - kerogen (CHR CREI)
  - molecular crystals for pharmacy

Research example: Anode for battery

PhD student **Roman Kapaev**: Chem Commun 56, 1541 (2020)

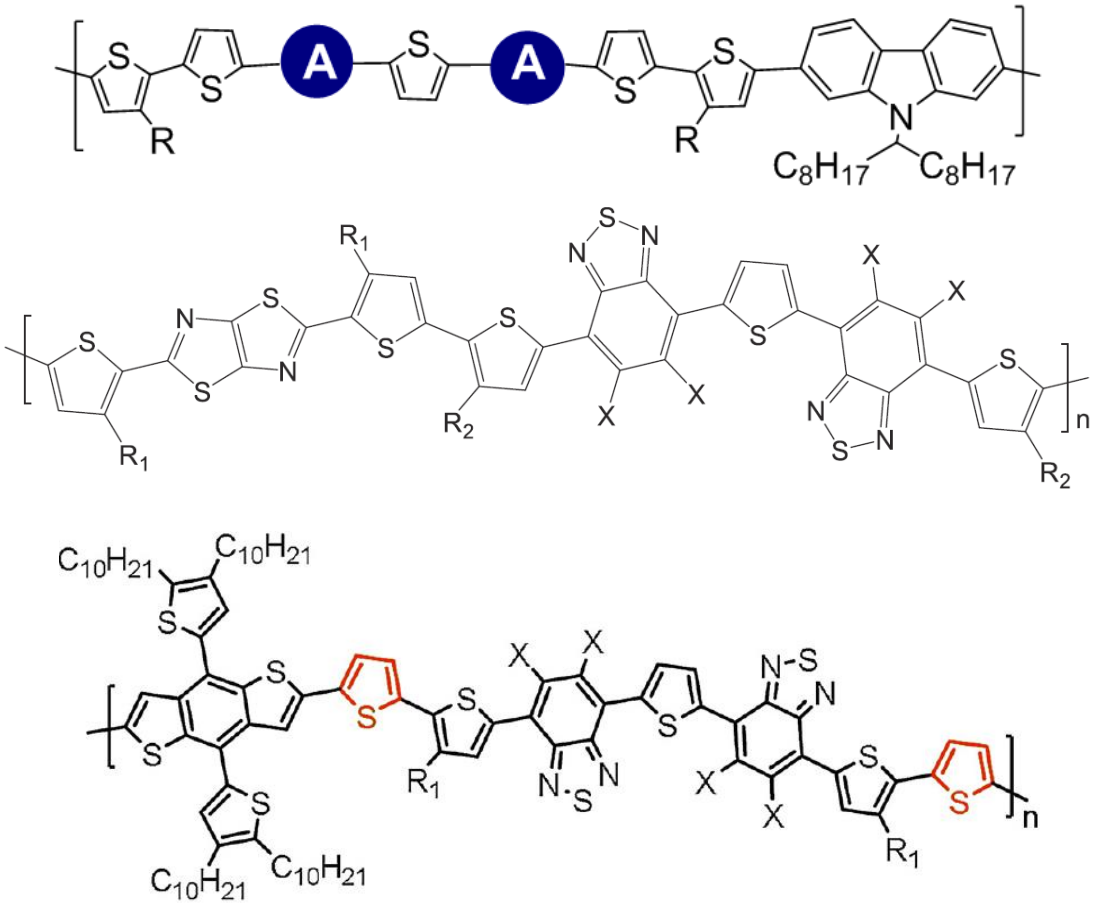
Comprehensive analysis of charge storage mechanisms of a π-d conjugated polymer for alkali-ion battery anodes



Research example: Solar cells

Pavel Troshin's Lab: Dyes and Pigments 185, 108899 (2021); Solar Energy 198, 605 (2020); Synthetic Metals 259, 116231 (2020)

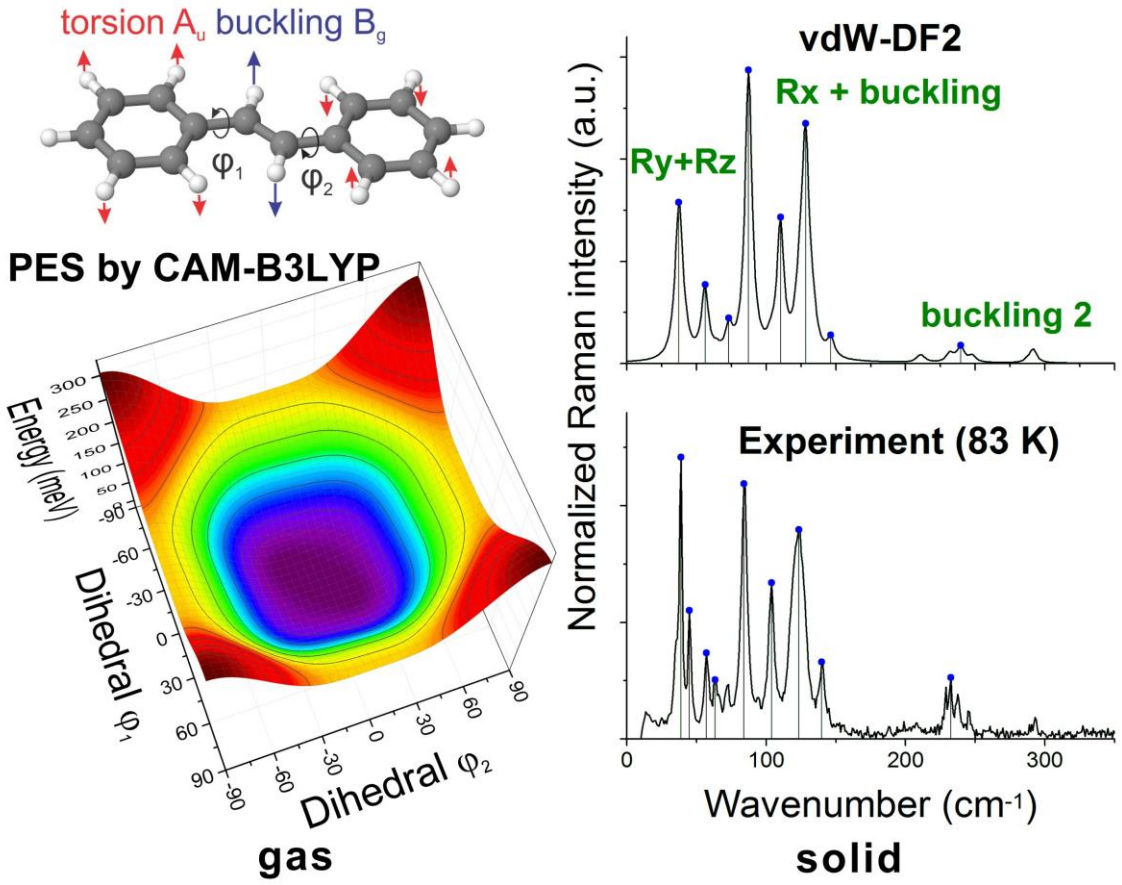
Combined experimental-theoretical study of donor-acceptor polymers for solar cells



Research example: Theoretical studies

Postdoc **Nikita Tukachev**: J Phys Chem Lett 10, 3232 (2019)

Unveiling puzzling details of molecular structure of stilbene



Course logistics

See course web-site at
http://zhugayevych.me/edu/Organic/index.htm

Read carefully:

- Syllabus
- Schedule
- Literature
- Assignments