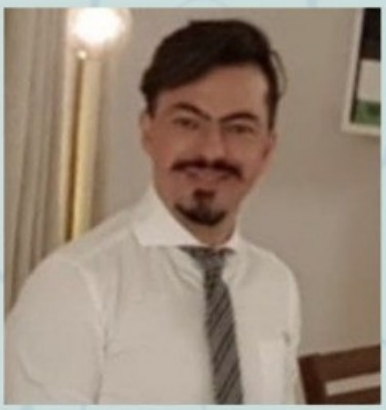
PROGRAMA DE PÓS GRADUAÇÃO EM FÍSICA

MINICURSO



Prof. Cleber Fabiano do Nascimento Marchiori

Karlstads Universitet, Suécia

"ADVANCED ORGANIC MATERIALS FOR ENERGY CONVERSION AND STORAGE"

DATAS:

1ª SEMANA: 09/11 A 12/11;
2ª SEMANA: 16/11 A 19/11;
3ª SEMANA: 23/11 A 26/11;

PARA MAIS INFORMAÇÕES:

Advanced Organic Materials for Energy Conversion and Storage

The aim of this course is to give an overview on the design and characterization of organic materials for energy related applications. Within the 4 weeks, different classes of materials as small molecules, copolymer and covalent frameworks (COFs) will be discussed as well as their applications as active layers in organic photovoltaic devices (OPVs), as photocatalysts for solar fuels production and as redox-active materials in organic batteries. Besides the materials development, the cutting-edge theoretical and experimental techniques applied to the characterization and design of novel materials will be presented.
The course will be structured as follow:

I. Course modules & Lectures:

Lecture 1 – *Organic Materials for energy related application – An overview*

The aim of this lecture is to give an overview of different classes of organic materials (at least some of them) that have been extensively studied for different "energy related application". A great deal of attention will be putted in some multifunctional materials which can be applied in different field such as OPVs, photocatalytic H_2 production and redox-active materials for Me-ion batteries (in particular Li-ion Batteries). This "inaugural" lecture will give a common ground for the more detailed and specific discussions that will be developed during the course.

Part I: Organic and Hybrid Photovoltaics

The first part of course will be dedicated to the latest developments regarding organic and hybrid photovoltaic devices. The purpose is to give an overview on the development timeline of materials using as active layer in OPVs and the recent developments regarding new device architectures and technological applications.

Lecture 2 – *OPV: developments of donor materials*

Lecture 3 – *OPV: developments of acceptor materials*

Lecture 4 – *OPV: devices architecture & novel concepts*

Lecture 5 – *Perovskites solar cells*

Part II: Organic Photocatalysts for Solar Fuel Production

In this module the application of organic materials as photocatalysts for solar fuels production will be discussed. For instance, the use of donor-acceptor copolymers as photocatalyst for H_2 evolution will be presented as well as the theoretical development in finding descriptors for a rational design of novel photocatalysts.

Lecture 6 – *Organic Photocatalysts H_2 evolution*

Lecture 7 – *Organic Photocatalysts for solar fuels production*

Part III: Organic Materials for Energy Storge: from electrodes to electrolytes

Although Li-ion batteries be a well-stablished technology, the issues related to the use of inorganic materials, as heavy metals, raises concerns regarding their recycling in the end of the life of the devices, besides being scarce and depended of mining processes. In this context, the use of organic redox active material raises as a very promising alternative for energy storage devices. In this module, the development on the design of small molecules and polymeric materials for Li-ion (amongst other chemistries) batteries will be presented as well as the use of solid polymer electrolytes for Li-metal batteries.

Lecture 8 – ***Organic Electrode Materials from Small molecules to Copolymers***

Lecture 9 – ***Solid Polymer Electrolytes***

Lecture 10 – ***Post-Lithium organic batteries***

Lecture 11 – ***Graphene based Batteries***

Part IV: Advanced tool for materials and devices characterization

In this module, advanced theoretical and experimental techniques applied to the design and characterization of organic materials will be presented. The materials modelling in a multiscale approach will be discussed as a strategy to reconcile macroscopic properties with atomistic modeling. Experimental advanced techniques applied to characterization of organic based materials and devices will be presented by specialists in the field.

Lecture 12 – ***Modelling Organic Materials: A Multiscale approach***

Lecture 13 – ***Modelling Organic Materials: An atomistic scale perspective***

Lecture 14 – ***Advanced Theoretical tools: MD and Monte Carlo***

Lecture 15 – ***Advanced Theoretical tools: Artificial Intelligence aided design of novel materials***

Lecture 16 – ***Advanced Spectroscopic techniques: AFM-IR***

Lecture 17 – ***Advanced Spectroscopies: In-situ and operando techniques***

Part I: Organic and Hybrid Photovoltaics

Juganta K. Roy, Supratik Kar & Jerzy Leszczynski (Editors), *Development of Solar Cells Theory and Experiment*, Springer 2021, DOI: https://doi.org/10.1007/978-3-030-69445-6

Karl Leo (Editor), *Elementary Processes in Organic Photovoltaics*, Springer 2017 DOI 10.1007/978-3-319-28338-8

Yongfang Li (Editor), *Organic Optoelectronic Materials*, Spinger 2015, DOI: 10.1007/978-3-319-16862-3

Part II: Organic Photocatalysts for Solar Fuel Production

Haining Tian, Gerrit Boschloo &Anders Hagfeldt (Editors), *Molecular Devices for Solar Energy Conversion and Storage*, Spinger 2018, DOI: https://doi.org/10.1007/978-981-10-5924-7

Part III: Organic Materials for Energy Storge: from electrodes to electrolytes

Masaki Yoshio, Ralph J. Brodd, Akiya Kozawa (Editors), *Lithium-Ion Batteries Science and Technologies*, Springer 2009, DOI: 10.1007/978-0-387-34445-4

Beta Writer, *Lithium-Ion Batteries A Machine-Generated Summary of Current Research*, Springer 2019, DOI: https://doi.org/10.1007/978-3-030-16800-1

ACTIVITIES SCHEDULE (44h)

Part I – Organic and Hybrid Photovoltaics

	TIME	Monday 08/11	Tuesday 09/11	Wednesday 10/11	Thursday 11/11	Friday 12/11
WEEK 1	08.00/08.40		**Electrodynamics II**	**Lecture 3**	**Electrodynamics II**	
	09.00/09.30		**Electrodynamics II**	**Lecture 3**	**Electrodynamics II**	
	09.45/10.30	**Quantum Physics II**	**Course Introduction**	**Quantum Physics II**		**Lecture 4**
	10.45/11.30	**Quantum Physics II**	**Lecture 1**	**Quantum Physics II**		**Lecture 5**
	14.00/14.45	**Statistical Physics**	**Lecture 2**	**Statistical Physics**		**Lecture 5**
	15.00/16.00	**Statistical Physics**	**Lecture 2**	**Statistical Physics**	Department Seminar	

Part II – Organic Photo(electro)catalysts for Solar Fuel Production
Part III – Organic Materials for Energy Storage

	TIME	Monday 15/11	Tuesday 16/11	Wednesday 17/11	Thursday 18/11	Friday 19/11
WEEK 2	08.00/08.40	Holyday	**Electrodynamics II**	**Lecture 8**	**Electrodynamics II**	**Lecture 9**
	09.00/09.30	Holyday	**Electrodynamics II**	**Lecture 8**	**Electrodynamics II**	**Lecture 9**
	09.30/10.30	**Quantum Physics II**	**Lecture 6**	**Quantum Physics II**	**Lecture 11**	**Lecture 10**
	09.45/11.30	**Quantum Physics II**	**Lecture 6**	**Quantum Physics II**	**Lecture 11**	**Lecture 10**
	14.00/14.45	**Statistical Physics**	**Lecture 7**	**Statistical Physics**		
	15.00/16.00	**Statistical Physics**	**Lecture 7**	**Statistical Physics**	Department Seminar	

Part IV – Advanced tool for materials and devices characterization

	TIME	Monday 22/11	Tuesday 23/11	Wednesday 24/11	Thursday 25/11	Friday 26/11
WEEK 3	08.00/08.40		**Electrodynamics II**		**Electrodynamics II**	**Lecture 16**
	09.00/09.30		**Electrodynamics II**		**Electrodynamics II**	**Lecture 16**
	09.30/10.30	**Quantum Physics II**		**Quantum Physics II**	**Lecture 14**	**Lecture 17**
	09.45/11.30	**Quantum Physics II**		**Quantum Physics II**	**Lecture 14**	**Lecture 17**
	14.00/14.45	**Statistical Physics**	**Lecture 12**	**Statistical Physics**	**Lecture 15**	
	15.00/16.00	**Statistical Physics**	**Lecture 13**	**Statistical Physics**	Department Seminar	