Theoretical Methods for Simulation of Materials

22.02.-05.03.2021

Coordination: Dr. Johannes Gierschner

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With the support of the Erasmus+ Programme of the European Union

European Master in Theoretical Chemistry and Computational Modelling EM-TCCM

2-year master (120 ECTS)

- fundamental quantum chemistry
- use & modify most advanced software codes
- simulate complex systems: QM & MD

M1: local level, common content

fundamental aspects: theoretical methodologies, computational techniques, main applications

M2: European level, common courses

- compulsory parts
- elective subjects

new module:

Theoretical Methods for Simulation of Materials

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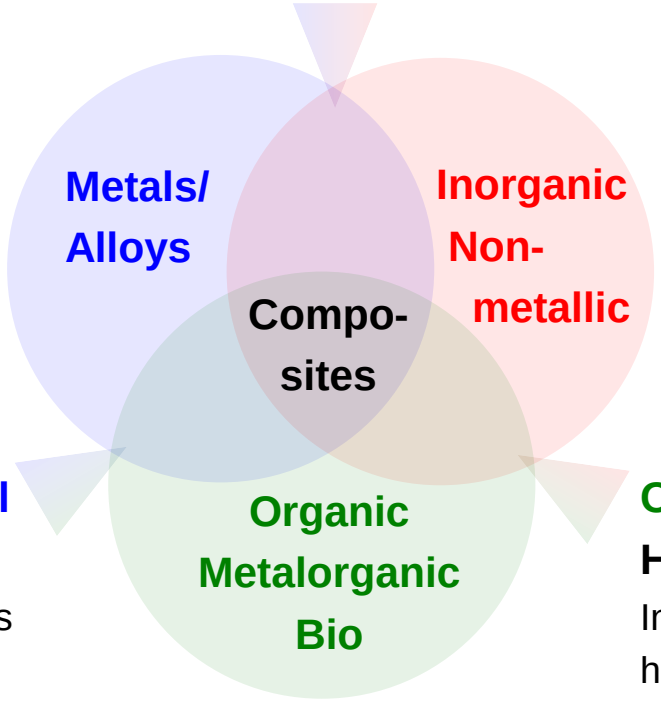
Semiconductor-Metal Hybrids
Interfaces, doping

solids
nanostructures



Ceramics: glasses, crystals
Semiconductors: crystals, quantum dots
2D Materials

Organic-Metal Hybrids
MOFs, Interfaces
Nandot-doping

Organic-Inorganic Hybrids
Interfaces, doping
host-guest compounds

Polymers: isolating (thermoplasts, thermosets, elastomers)
semi-conducting, COFs
Molecular solids (crystalline, amorphous)
Org.-Org. interfaces/mixtures/host-guest comp./cocrystals
Carbon Allotropes
Biomaterials (membranes, proteins, drugs, co-pigments)

Properties

with response to...

- Mechanical (force)
- Chemical (stability)
- Electrical
- Magnetic
- Thermal
- Electromagnetic
  - NMR, MW, IR
  - UV/Vis (Abs, Reflect, Scatter., Luminescence)

Applications

- Semi-/conductors
- Energy Storage
- (Photo-)Catalysis
- LEDs
- Photovoltaics
- Senisng
- Lasing...

Materials Science: an interdisciplinary field...

Aspects

- Material Synthesis
- Materials Characterization
- Material preparation:
  thin film, nanoparticle suspension/deposition, crystal etc...
- Device Engineering
- Spectroscopy:
  NMR, MW, IR, UV/Vis Abs, PL, TA etc..
- Electrical Measurements
- Modelling

...

Fields

- Chemistry:
  Inorganic/Organic/Bio-/ Materials/Physical/Theoretical
- Physics:
  Solid State/Theoretical
- Biology, Medicine
- Engineering...

...a challenge for students in quantum chemistry/ computational modelling...

"Electrons in Solids"

"Targeted Mat. Design"

"Nanomaterials: a view from experimental...

...Physics"

...Chemistry"

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Coord.

Johannes Gierschner
Madrid

Lecturers

Pere Alemany
Barcelona

Rodolfo Miranda
IMDEA
Madrid

Nazario Martín
UCM/IMDEA
Madrid

Jerôme Cornil
U. Mons

Patrick Trouillas
U. Limoges

Hands-On

Javier Junquera
U. Cantabria
Santander

Michele Pisarra
UAM
Madrid

Francisco Guinea
IMDEA
Madrid

Michal Otyepka
U. Palacky
Olomouc

Monica Calatayud
U. Sorbonne
Paris

Julen Munárriz
U. Oviedo

Alejandro Gaita
U. Valencia

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Program

A. Preparation Course (*non-mandatory*)

Electrons in Solids 18.02.2021

Pere Alemany, Univ. Barcelona 4h

B. Lectures

Introduction

Targeted Materials Design

Johannes Gierschner,

IMDEA Nanoscience, Madrid 1h

An Experimental View on Materials

Nano-Materials:

a view from Experimental Physics

Rodolfo Miranda,

IMDEA Nanoscience, Madrid 2h

Nano-Materials:

a view from Experimental Chemistry

Nazario Martín,

IMDEA Nanoscience & UCM, Madrid 2h

Organic Materials

Organic Semiconductors for Optoelectronics

Jerôme Cornil, Univ. Mons 5h

Graphene and 2D Materials

Graphene and 2D Materials

Francisco Guinea, IMDEA Nanoscience, Madrid 2h

Physicochemical Aspects of 2D Materials

Michal Otyepka, Univ. Olomouc 2h

BioMaterials

Basic Knowledge & Applications / Modelling Biomembranes

Patrick Trouillas, Univ. Limoges 4h

Inorganic Materials & Interfaces

Modelling Ideal and Complex Surfaces for Catalytic Applications

Monica Calatayud, Univ. Sorbonne, Paris 2h

Perovskites Modelling

Julen Munarriz, Univ. Oviedo 1h

Spin Qubits and the So-Called 2nd Quantum Revolution: the Role of TCCM

Alejandro Gaita, ICMol, Valencia 3h

C. Hands-On Courses

SIESTA: Calculations of Inorganic Semiconductors

Javier Junquera, Univ. Cantabria, Santander 8h

VASP: Calculations of 2D materials, Organic Layers & Crystals

Michele Pisarra, IMDEA Nanoscience & UAM, Madrid 8h

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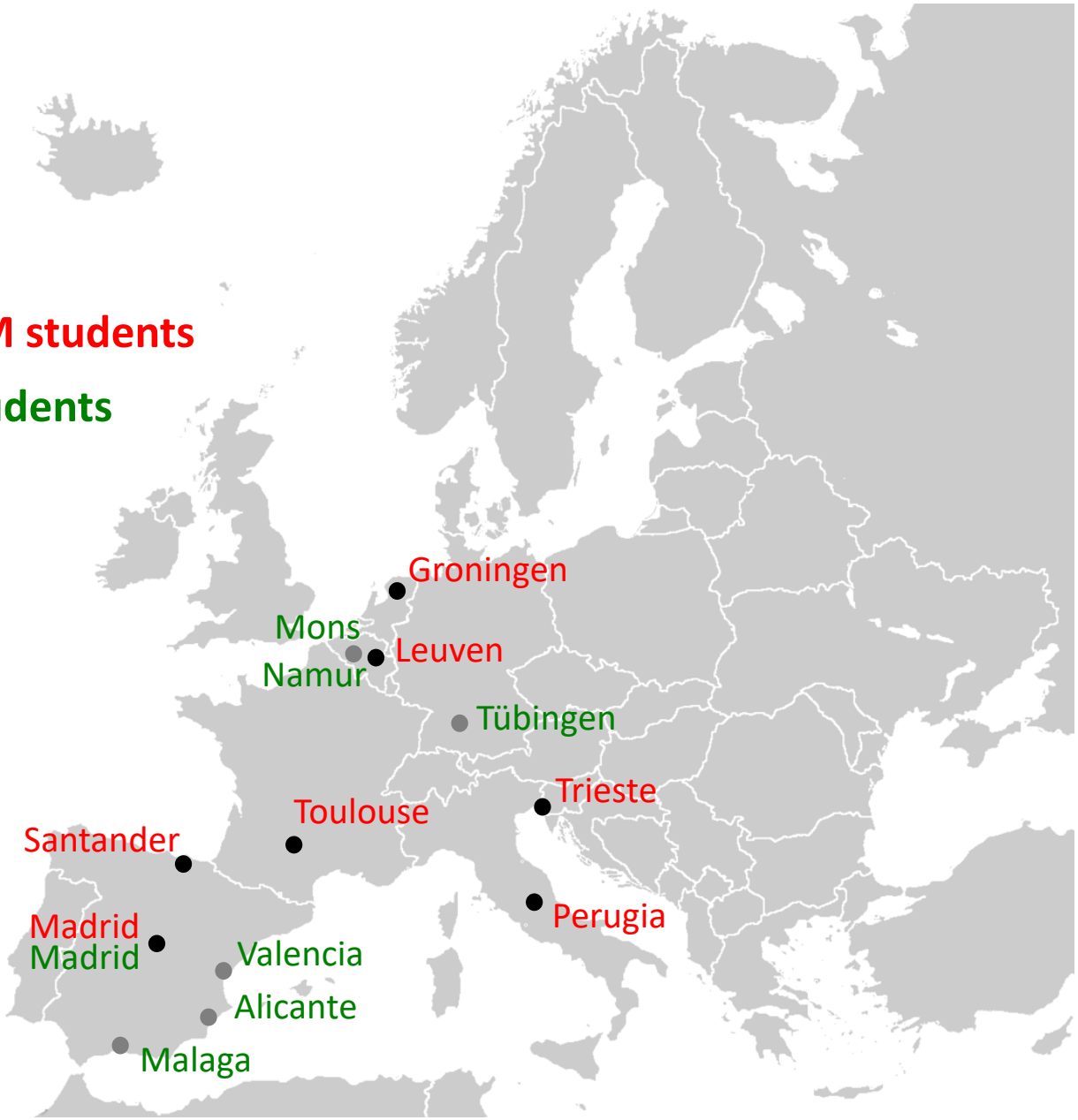
12 EM TCCM students

16 guest students



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Prep. Course	Thu, 18.02.
11:00-12:00	**Elect. in Solids** P. Alemany
12:00-13:00	P. Alemany
lunch break	
15:00-16:00	P. Alemany
16:00-17:00	P. Alemany

Week 1	Mon, 22.02.	Tue, 23.02.	Wed, 24.02.	Thu, 25.02.	Fr, 26.02.
09:45-10:45	**Introduction** J. Gierschner	**Organic Mat.** J. Cornil			
coffee break					
11:00-12:00	**Exp. View 1** R. Miranda	J. Cornil	**2D Mat. 1** F.Guinea	**Inorg. Mat. 1** M. Calatayud	**Spin Qubits** A. Gaita
12:00-13:00	R. Miranda	J. Cornil	F.Guinea	M. Calatayud	A. Gaita
lunch break					
15:00-16:00	**Exp. View 2** N. Martín	J. Cornil	**2D Mat. 2** M. Otyepka	**Inorg. Mat. 2** J. Munarriz	A. Gaita
16:00-17:00	N. Martín	J. Cornil	M. Otyepka		

Week 2	Mon, 01.03.	Tue, 02.03.	Wed, 03.03.	Thu, 04.03.	Fr, 05.03.
11:00-12:00	**Bio-Mat.** P. Trouillas	**Hands-On 1** J. Junquera	**Hands-On 1** J. Junquera	**Hands-On 2** M. Pisarra	**Hands-On 2** M. Pisarra
12:00-13:00	P. Trouillas	J. Junquera	J. Junquera	M. Pisarra	M. Pisarra
lunch break					
15:00-16:00	P. Trouillas	J. Junquera	J. Junquera	M. Pisarra	M. Pisarra
16:00-17:00	P. Trouillas	J. Junquera	J. Junquera	M. Pisarra	M. Pisarra