UNIVERSIDAD AUTÓNOMA DE MADRID

31248 - SOLIDS

Syllabus Information

Code - Course title: 31248 - SOLIDS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Solids

1.2.Course nature

Optional

1.3.Course level

Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

a. Subject´s coordinator:
- Name and surname: Antonio M. Márquez Cruz
- Email: marquez@us.es
- Institution: University of Sevilla
- Department: Physical Chemistry

b. Lecturer:
- Name and surname: Pablo García Fernández
- Email: garciapa@unican.es
- Institution: University of Cantabria
- Department: Earth Sciences and Physics of Condensed Matter

c. Lecturer:
- Name and surname: Cristina Díaz Blanco
- Email: cristina.diaz@uam.es
- Institution: Universidad Autónoma de Madrid
- Department: Chemistry

d. Lecturer:
- Name and surname: Julia Contreras García
- Email: julia.contreras.garcia@gmail.com
- Institution: Pierre et Marie Curie
- Department: Theoretical Chemistry

e. Lecturer:
- Name and surname: Coen de Graaf
- Email: coen.degraaf@urv.cat
- Institution: Universidad Rovira i Virgili
- Department: Physical and Inorganic Chemistry

f. Master's coordinators:
- Manuel Alcamí: manuel.alcami@uam.es
- Sergio Díaz-Tendero: sergio.diaztendero@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.

CG01 - Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.

CG04 - Students develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.

CROSS-COMPREHENSIVE COMPETENCES

CT03 - Students have the ability of analyze and synthesize in such a way that they can understand, interpret and evaluate the relevant information by assuming with responsibility their own learning or, in the future, the identification of professional exits and employment fields.

SPECIFIC COMPETENCES

CE03 – Students acquire an overview of the different applications of the Theoretical Chemistry and modeling in the fields of Chemistry, Biochemistry, Materials Sciences, Astrophysics and Catalysis.

CE04 - Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.

CE28 - Provide basic methodology for the treatment of periodic systems, crystals and polymers

1.12.2.Learning outcomes

To provide to the students the basic methodology to treat pure and defective periodic systems of condensed matter dealing with the following topics: Crystallography; Electronic structure; Thermodynamics; Phase transitions; Surfaces; Heterogeneous catalysis; Optical properties in condensed matter; Magnetism. In the course the students will receive an intensive introduction to the modelization and treatment of all these issues in solids.

1.13.Course contents

1. CRYSTALLOGRAPHY

1.1 Symmetry in crystals

1.2 Reciprocal space

2. ELECTRONIC STRUCTURE

2.1 Cluster and periodic models

2.2 Computational methodologies

3. THERMODYNAMICS

3.1 Static approximation and thermal models

3.2 Phase transitions

4. CHEMICAL BONDING

4.1 Scalar field induced topologies in crystals

4.2 Characterization of chemical bonding in solids and relationship to macroscopic properties

5. AB INITIO ELECTRONIC STRUCTURE CALCULATIONS IN SOLIDS

5.1 Comparison of wave function and density functional methods

5.2 From crystallographic data basis to electronic structure calculations

6. THERMODYNAMIC PROPERTIES OF CRYSTALLINE SOLIDS

6.1 E(V) curves and the static model

6.2 Phonons in crystals

7. AB INITIO SIMULATIONS OF STRUCTURAL, THERMODYNAMIC PROPERTIES AND REACTIVITY IN SURFACES

8.1 Cluster and periodic models

8.3 Surface structure and reconstruction

8.2 Adsorption and reactivity in surfaces

8. OPTICAL PROPERTIES

8.1 Quantum chemistry and the macroscopic Maxwell equations

8.2 Applications

9. ELEMENTS OF MOLECULAR AND CRYSTALLINE MAGNETISM

9.1 Model and effective hamiltonians

9.2 Applications

1.14.Course bibliography

[01] L. Kantorovich, "Quantum Theory of the Solid State" (Kluwer, Dordrecht, The Netherlands, 2004).

[02] R. M. Martin, "Electronic Structure: Basic theory and practical methods" (Cambridge UP, Cambridge, UK, 2004).

[03] E. Kaxiras, "Atomic and Electronic Structure of Solids" (Cambridge UP, Cambridge, UK, 2003).

[04] O. Anderson, "Equations of State for Solids in Geophysics and Ceramic Science" (Oxford UP, Oxford, UK, 1995).

[05] A. Otero-de-la-Roza and V. Luaña, "Equations of state and thermodynamics of solids using empirical corrections in the quasiharmonic approximation", Phys. Rev. B 84 (2011) 024109.

[06] A. R. Oganov, Ed, "Modern methods of crystal structure prediction" (Wiley-VCH, 2011).

[07] J. P. Poirier, "Introduction to the Physics of the Earth's Interior" (Cambridge UP, Cambridge, UK, 2000).

[08] B. Bersuker, "The Jahn-Teller effect" (Cambridge UP, Cambridge, UK, 2006).

[09] E. R. Johnson, S. Keinan, P. Mori-Sanchez, J. Contreras-Garcia, A. J. Cohen, and W. Yang, “Revealing Noncovalent

Interactions", J. Am. Chem. Soc. 132 , 6498 (2010)

[10] B. Silvi, A. Savin, "Classification of chemical bonds based on the topological analysis of electron localization functions", Nature 371, 683 (1994)

[11] J. Contreras-Garcia, A. M. Pendas, B. Silvi, J. M. Recio, "Computation of local and global properties of the ELF topology in crystals", J. Theor. Chem. Comp. 113, 1068 (2009)

[12] A. Otero-de-la-Roza, J. Contreras-Garcia, E. R. Johnson, "Revealing non-covalent interactions in solids, NCI plots revisited" Phys. Chem. Chem. Phys. 14, 12165 (2012)

[13] P. García-Fernández, J. Wojdel, J. Iñiguez and J. Junquera "Second-principles method for materials simulations including electron and lattice degrees of freedom" Phys. Rev. B 93, 195137 (2016)

[14] M. S. Dresselhaus, G. Dresselhaus, A. Jorio "Group Theory: Applications to the Physics of Condensed Matter" (Springer, 2007)

[15] J.L. Whitten and H. Yang, "Theory of Chemisorption and reactions on metal surfaces" Surf. Sci. rep. 24, 59 (1996)

[16] A. R. Leach, "Molecular modeling" (Prentice Hall, 2001).

[17] T. Schlick,"Molecular modeling and simulation" (Springer, 2002).

[18] D. Marx and J. Hutter, "Ab initio molecular dynamics: Theory and implementation", in "Modern methods and algorithms on quantum chemistry" by J. Grotendorst (Ed.), (John von Neumann Institute, NIC series vol. 1 \& 3, 2000).

[19] C. Fiolhais, F. Nogueira and M. A. L. Marques, Eds. "A Primer in Density Functional Theory", (Springer, Heidelberg, 2003).

[20] R. Dronskowski "Computational Chemistry of Solid State Materials" (Wiley-VCH, 2005).

[21] P. Huang, and E. A. Carter, "Advances in Correlated Electronic Structure Methods for Solids, Surfaces and Nanostructures", Ann. Rev. Phys. Chem. 59 (2008) 261.

[22] G. Pacchioni, A. M. Ferrari, A. M. Márquez, and F. Illas, "Importance of Madelung Potential in Quantum Chemical Modeling of Ionic Surfaces", J. Comput. Chem. 18 (1997) 617.

[23] J. N. Norskov, F. Abild-Pedersen, F. Studt, and T. Bligaard "Density functional theory in surface chemistry and catalysis" PNAS 108 (2011) 937-943.

[24] F. Yang, J. Graciani, J. Evans, P. Liu, J. Hrbek, J. Fernández. Sanz, and J. A. Rodríguez, "CO oxidation on inverse CeOx/Cu(111) Catalysts: High catalytic activity and ceria-promoted dissociation of O2", J. Am. Chem. Soc. 133 (2011) 3444.

[25] C. de Graaf, R. Broer, "Magnetic Interactions in Molecules and Solids" Second volume of the textbooks of the TCCM Master. (Springer 2015).

[26] J. P. Malrieu, R. Caballol, C. J. Calzado, C. de Graaf, N. Guihéry "Magnetic Interactions in Molecules and Highly Correlated Materials: Physical Content, Analytical Derivation, and Rigorous Extraction of Magnetic Hamiltonians", Chemical Reviews 114, 429-492 (2014).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	50
Independent study time	75

2.2.List of training activities

Activity	# hours
Lectures	50
Seminars	
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

Lecture: The Professor will deliver lectures about the theoretical contents of the course during two-hour sessions. The presentations will be based on the different materials available at the Moodle platform.

Network teaching: All the tools available at the Moodle website (https://posgrado.uam.es) will be used (uploading of teaching

materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

Solving practical exercises: Numerical problems, multiple choice questions, interpretation and information processing, evaluation of scientific publications, etc..

Written reports: Orientation and supervision in the preparation of written reports.

3.Evaluation procedures and weight of components in the final grade

3.1.Regular assessment

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on exercises that must be done during the course. The next criteria will be followed for assessment of student exercises:

- 60% from a practical exam on the course contents and practical session,
- 20% from discussions between the student and professor in tutoring sessions and seminars.
- 20 % from writing an essay based on a scientific paper.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	60
Continuous assessment	40

3.2.Resit

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

4.Proposed workplan

Please, check the official schedule posted on the master website.