



# Thermodynamics and defects of solids



Niveau d'étude  
BAC +4



ECTS  
5 crédits



Composante  
Faculté des  
Sciences

## En bref

- > **Date de début des cours:** 1 sept. 2021
- > **Langue(s) d'enseignement:** Anglais
- > **Méthode d'enseignement:** En présence
- > **Organisation de l'enseignement:** Formation initiale
- > **Ouvert aux étudiants en échange:** Non

## Présentation

### Description

This module is devoted to deliver basic knowledge on the thermodynamics of defects. The understanding and basic concepts of defects in stoichiometric and non-stoichiometric solids is an important aspect to better understand and design materials for ionic and electronic conductivity with a specific relevance for energy materials. The lecture introduces and discusses the nature of point defects which intrude upon the perfect geometry of ideal crystal structures:

- \* Introduction into point defects (missing or misplaced atoms, ions or electrons)
- \* Discussion of thermodynamic concepts of order-disorder phenomena in solid solutions

- \* Understanding of Brouwer diagrams for oxides in order to emphasize the role of surrounding atmosphere onto the defect equilibrium at high temperature.
- \* Understanding of diffusion pathways and energies of ions and electrons, as a major consequence of point defects, giving rise to electrical transport is investigated for ionic conductors.
- \* Experimental investigations of measuring the ionic conductivity versus the temperature are described. The method of Impedance Spectroscopy Measurements is discussed.
- \* Presentation of the Kröger-Vink Notation of defects
- \* Mott-Hubbard insulators

Volumes horaires\* :

CM : 24

TD : 12

### Objectifs

The understanding of the role of point defects in solid on the transport properties and the structural stability.

To apply the concept of Brouwer diagram to control the conductivity in oxides.

Electronic and ionic conductivity in metallic oxides

Understanding concepts of ceramic semiconductors

### Contrôle des connaissances



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## Syllabus

- Ceramic (oxide) materials with metallic conductivity
- Defect chemistry (explaining properties of semiconductors and ionic conductors)
- Crystal-field splitting of d-orbitals
- Strong electron correlation (Coulomb repulsion)
- Structure instabilities (Peierls distortion)
- Anderson localization (electron localization when impurities or defects concentration is large )
- Mott-Hubbard insulators
- Ceramic semiconductors
- point defects
- extended defects
- Presentation of the Kröger-Vink Notation of defects
- Ionic conductors. Solid oxide fuel cells. Batteries.
- Brouwer diagrams and defect equilibrium at high temperature
- Understanding of diffusion pathways and energies of ions and electrons, as a major consequence of point defects, giving rise to electrical transport is investigated for ionic conductors.
- Experimental investigations of measuring the ionic conductivity versus the temperature via Impedance Spectroscopy Measurements

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## Infos pratiques

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### Contacts

Responsable pédagogique

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### Lieu(x)

➤ Montpellier - Triolet

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## Informations complémentaires