



## **APDIC report 2022**

French contribution

Jean-Marc Joubert

15<sup>th</sup> June 2023

### **1. Group activities in 2022**

The recently created Association Française de Thermodynamique des Matériaux (AFTherMat, French Association for Thermodynamic of Materials) entered in its second year of existence and now has 110 formal members. The Board of Directors is composed by Olivier Dezellus (President), Jean-Marc Joubert (Treasurer) and Sophie Schuller (Secretary).

We gather all the French activities on the thermodynamic of the materials at high temperature, including a significant contribution to the phase diagrams of alloys and ceramics and a lot of activities on glasses.

A poster representing the activities of our group was created and is reproduced at the end of this document.

The annual meeting took place in October 2022 in Lille in the frame of the conference Matériaux 2022, at which we managed to have a special session dedicated to phase transformations and thermodynamics.

AFTherMat is still following the activities, as a foreign participant, of the Thermodynamic Consortium (ThermoCon) of Alexandra Navrotsky. Christophe Drouet (Cirimat, Toulouse) represents the association to the ThermoCon meetings. <https://www.thermocon.org/>

We are members of two important societies : the French Materials Federation (FFM, <https://www.ffmateriaux.org/>) and National Network of Metallurgy (RNM, <https://www.rnm-metallurgie.fr/>).

We have launched, a series of online seminars. These are recorded and available on our Youtube channel (@afthermat3308).

N°1 – March 2022 : Phase diagram of the Cr-Mn system studied by in-situ powder neutron diffraction

Jean-Marc JOUBERT (ICMPE)

<https://youtu.be/9xjq4MyqV8c>

N°2 – October 2022 : Thermodynamique des phases gazeuses

Ioana NUTA (SIMaP)

[https://youtu.be/36\\_QEXMSiLc](https://youtu.be/36_QEXMSiLc)

N°3 – November 2022 : Apport de la thermodynamique et des diagrammes pour la compréhension des évolutions structurales des alliages Zr

Caroline TOFFOLON (CEA)

<https://youtu.be/8zMvPE8cGCA>

N°4 – December 2022 : La lévitation aérodynamique à haute température comme outil de synthèse et de caractérisation au CEMHTI : usage, atouts et limites

Emmanuel DE BILBAO, Emmanuel VERON, Vincent SAROU-KANIAN (CEMHTI)

<https://youtu.be/5vFMFqjzv-A>

N°5 – January 2023 : L'entropie de configuration des verres

Daniel NEUVILLE IPGP : Institut de Physique du Globe de Paris

<https://www.youtube.com/watch?v=glyHopEAG6s>

N°6 - March 2023 : Modélisation de l'interdiffusion dans les matériaux métalliques

Thomas GHENO - (ONERA)

<https://www.youtube.com/watch?v=Wela7HDb-pE>

N°7 – April 2023 : Le concept de chemin de diffusion

Olivier Dezellus (Laboratoire des Multimatériaux et Interfaces, UMR CNRS – 5615, Université de Lyon 1)

<https://www.youtube.com/watch?v=y9D0plpKHRY>

N°8 – May 2023 : Les transitions Ordre/Désordre à partir de NACEF

Jean Marc FIORANI (Institut Jean Lamour, Université de Lorraine)

<https://www.youtube.com/watch?v=-CAYnzYsJMA>

N°9 – Juin 2023 : Les bases de l'analyse thermique # partie 1

Pierre BENIGNI (CNRS, IM2NP, Université Aix Marseille)

<https://www.youtube.com/watch?v= uzAGihhuCc>

We have also reinforced our teaching activities. We organized two in person formations on:

- Analysis of X-ray diffraction data and Rietveld analysis (3 days, January 2023, 20 persons)
- Thermo-Calc for beginners (2 days, January 2023, 20 persons)
- Thermodynamic calculations in the frame as a post-conference formation after the Métallurgie Quel Avenir ! conference (<https://metav2023.sciencesconf.org/>).

## **2. Website development**

Our new website <https://www.afthermat.fr/> is not yet fully operational. In the meantime, the old website is still available: <https://www.thermatht.fr/>

It contains:

- job offers: <https://www.thermatht.fr/offres-demploi/>
- useful pages containing tutorials or description of instrumental methods. We can highlight new pages on:
  - o experimental measurement of thermodynamic properties at high temperature: <https://www.thermatht.fr/methodes-experimentales-de-la-thermodynamique-des-materiaux-a-hautes-temperatures/>
  - o mass spectroscopy: <https://www.thermatht.fr/spectrometrie-de-masse-a-haute-temperature/>
  - o tutorial on the Rietveld method: <https://www.thermatht.fr/conduite-dun-affinement-par-la-methode-de-rietveld/>
  - o the Calphad method: <https://www.thermatht.fr/modelisation-thermodynamique-par-la-methode-calphad/>
  - o list of sources for thermodynamic data: <https://www.thermatht.fr/sources-de-donnees-thermodynamiques/>
  - o reference books: <https://www.thermatht.fr/ouvrages-de-reference/>
  - o useful links: <https://www.thermatht.fr/liens-incontournables/>
- a facility is available representing a skill inventory of the different members of the GdR/association. It can be found at <https://www.thermatht.fr/bdd-liste-enregistrements/>. A search can be made according to different criteria like skills, or systems of interest.

The website is in French, but many pages are easily understandable.

## **3. Main events related to Phase Diagrams in France in 2021**

### **3.1. SATA school**

For the fourth time, the School on Advanced Thermodynamic Assessment (SATA) was held in France (Toulouse) organized by the CIRIMAT laboratory of Toulouse (E. Epifano, A. Vande Put, D. Connétable, M. Dehmas and C. Drouet). The school gathered participants from all over the world. It consists of a complete training and practice thermodynamic optimization using the Parrot module of Thermo-Calc. Next edition is foreseen for 2024.

### 3.2. Conference Matériaux 2022

Matériaux is the largest French conference on materials. It is held every 4 years. It was organized in Lille, October 24-28, 2022. The influence of our group made it possible to have a dedicated session on phase transformations and thermodynamics. <https://materiaux2022.org/>

### 3.3 French-German speaking workshop

The second French-German-Austrian meeting on thermodynamics and kinetics of materials was held in Karlsruhe, February 2-3, 2023, organized by Hans Seifert and Stephanie Lippmann. It gathered almost 50 persons.

### 3.4. GdR IAMAT

We should mention the creation of the Network of Research IAMAT on Artificial Intelligence in Materials Science <https://iamat.cnrs.fr/>. We will maintain close relationship with our group.

## **4. Upcoming events in 2023**

### 4.1. Book: Thermodynamic data: from acquisition to application (in French)

In line with our thermodynamic school, a book will be published containing lectures and exercises on different subjects like calorimetry, thermal analysis, ab initio calculations, phase diagram determination, Calphad modeling...

### 4.2. Summer school on High Entropy Alloys

A summer school on high entropy alloys will be organized in Cargese (Corsica), 10<sup>th</sup>-16<sup>th</sup> September A special session will be dedicated to thermodynamic calculations including training.

### 4.3. Thermo-Calc user meeting

The French Thermo-Calc user meeting will be organized in Lyon 23<sup>rd</sup>-24<sup>th</sup> October thanks to Olivier Dezellus.

### 4.4. Annual meeting

Our annual meeting will take place in Orléans, 9<sup>th</sup>-10<sup>th</sup> November, organized by E. De Bilbao.

### 4.5. TOFA

The Thermodynamic OF Alloys conference will be held in Lyon, 23<sup>rd</sup>-27<sup>th</sup> September 2024, organized by O. Dezellus. <https://tofa2024.univ-lyon1.fr>

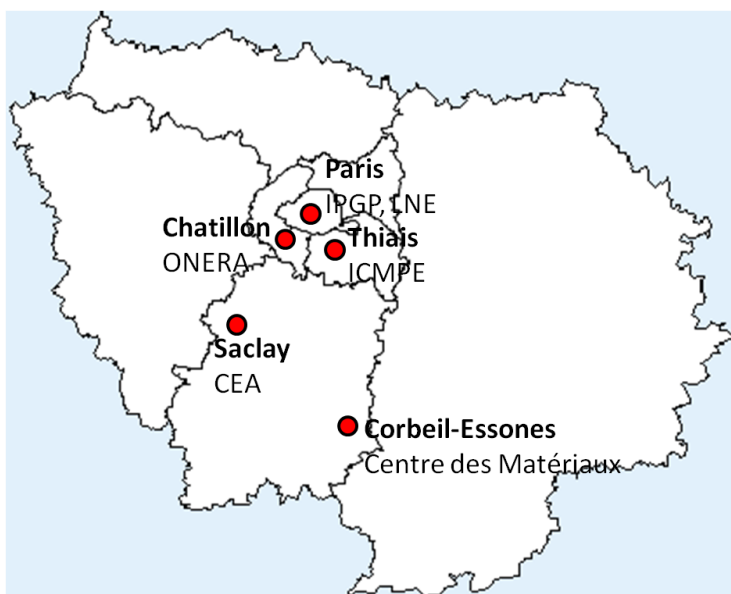
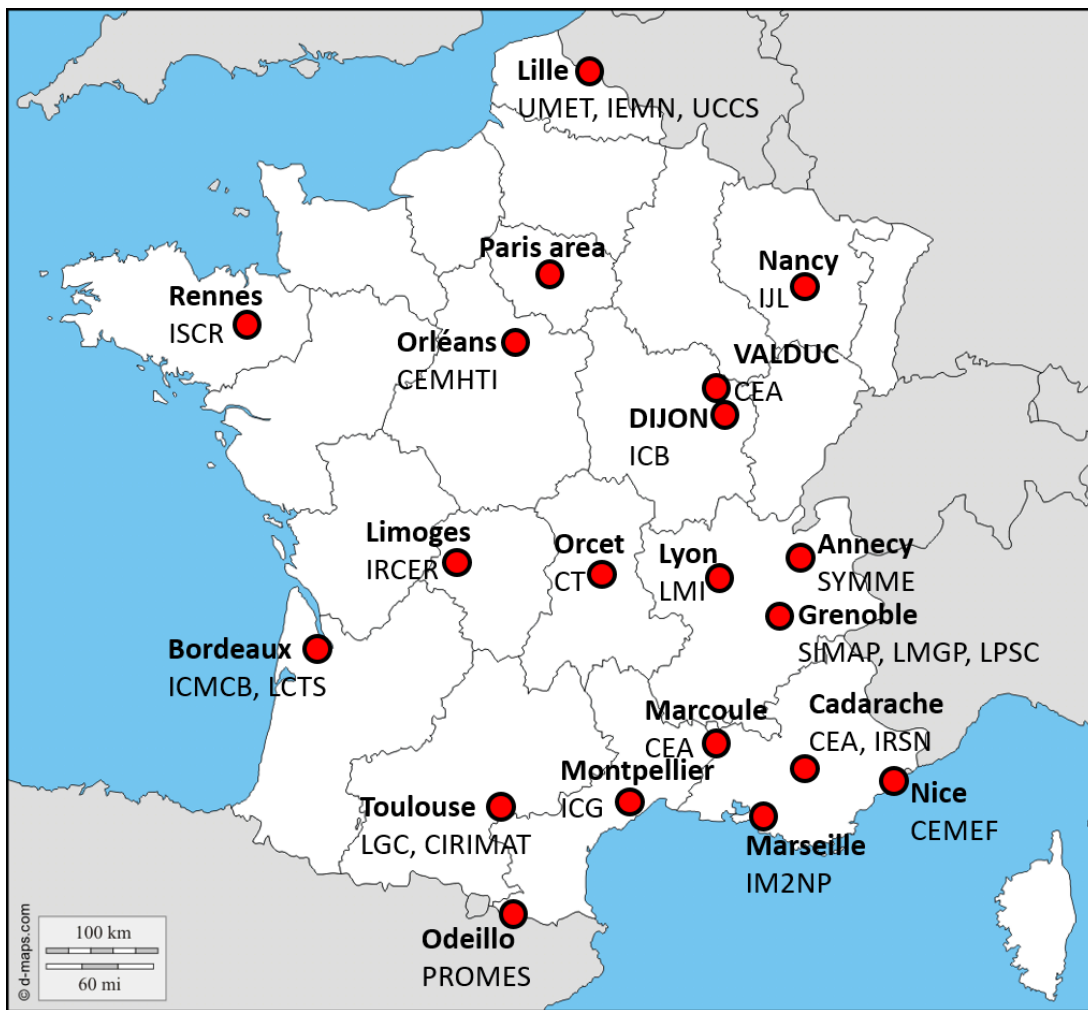
## **5. List of members of the AFtherMat association with affiliation and contact**

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Maps indicating the localization of the different research centers in France and in Paris area:







# AFTherMat

Association Française de Thermodynamique des Matériaux

Association loi 1901, created in 2021, whose purpose is to contribute to the development and dissemination of knowledge in the field of thermodynamics of materials. Its aim is to contribute to the advancement of research and technology in thermodynamics for the benefit of the French-speaking community..

## WHO ARE WE ?

More than 100 members:

- academics, students,
- industrials (nuclear, metallurgy, ceramics, materials for energetic transition...)

## JOIN US !

<https://www.afthermat.fr/>

## BOARD & COUNCIL

Administration council of 12 people

Board:

- President : Olivier Dezellus
- Treasurer : Jean-Marc Joubert
- Secretary : Sophie Schuller

## phase diagrams

Heat capacity  
thermodynamic measurements  
glass  
intermetallic compounds  
Nuclear  
phase equilibria  
alloys  
diffusion  
metallurgy  
thermodynamics  
Calorimetry  
ceramics  
Calphad  
Artificial Intelligence  
DFT calculation

## ACTIONS

### Courses

- Crystallography, Rietveld method (yearly)
- ThermoCalc for beginners (yearly)
- ThermoCalc: applications (La Métallurgie quel Avenir 2023)
- Thermodynamic for specific summer schools (HEA 2023)

### Dissemination

- Webinars (experimental methods, thermodynamic models, calculations, applications...): Youtube channel



Afthermat  
@afthermat3308 34 abonnés 9 vidéos  
Chaîne de l'Association Française de Thermodynamique des Matériaux >

- Yearly seminar of AFTherMat

## NETWORK

AFTherMat is proudly member of



FÉDÉRATION  
FRANÇAISE  
DES MATÉRIAUX

