



## **APDIC report 2019**

French contribution

Jean-Marc Joubert

20<sup>th</sup> May 2020

### **1. Presentation of the group**

GdR TherMatHT (<https://www.thermatht.fr/>) is the formal French representative and member of the APDIC. It is a Research Network (Groupement de Recherche) labelled by the CNRS existing since January 2013. It is headed by Olivier Dezellus and gathers 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. Approximately 140 people, mainly academics but also belonging to industry, are affiliated to the GdR.

### **2. Group activities in 2019**

Since 2018, we have had an internal call dedicated to finance internal research collaborative projects involving, in particular, younger researchers (internship, PhD students, post-docs). Two projects were financed in 2019 and the call was reopened in 2020 with two other projects funded (5k€ / project).

The Annual meeting of the GdR TherMatHT was held in Grenoble January 24-25, 2019, gathering about 50 people: <https://thermatht6.sciencesconf.org/>

For the first time, the meeting was preceded by a basic training school to Thermo-Calc and thermodynamic modelling (3 days) with more than 30 attendees. The school was held again in January 2020.

The GdR TherMatHT has made a formal subscription as a foreign participant to the Thermodynamic Consortium (ThermoCon) of Alexandra Navrotsky. Christophe Drouet (Cirimat, Toulouse) represents the GdR to the ThermoCon meetings. <https://www.thermocon.org/>

A bibliographic library is available gathering all the publications made by the group. It can be alimented and viewed at [https://hal.archives-ouvertes.fr/GDR\\_THERMATHT/](https://hal.archives-ouvertes.fr/GDR_THERMATHT/)

At the present time, 5 working groups are active with the following subjects:

- calculations (DFT and Calphad)
- high temperature measurements
- metallurgy
- silicon carbides
- thermodynamics of glass

### **3. Website development**

A lot of efforts have been put in the development of our website: <https://www.thermatht.fr/>

It contains now:

- 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 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. 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.

### **4. Main events related to Phase Diagrams in France in 2019**

#### **4.1. Conference La Métallurgie Quel Avenir ! (Metallurgy, what a future !)**

A conference on Metallurgy has been held in Nancy, 8-12 April 2019. <https://sf2m.fr/events/la-metallurgie-quel-avenir/>

#### **4.2 School Thermodynamic of Glass**

The School Thermodynamic of Glass is a workshop organized with the GdR TherMatHT, the ICG laboratory (Montpellier) and the German Glass Society (Deutsche Glastechnische Gesellschaft). It was organized in Erlangen by R. Conradt, N. Vedidsheva, D. R. Neuville and D. de Ligny 12<sup>th</sup> May 2019 with 40 participants among which 30 students.

### 4.3 IUPAC congress

The IUPAC congress was organized in Paris 5<sup>th</sup>-12<sup>th</sup> July 2019.

### 4.4 Workshop on the contribution of thermodynamic data

A meeting day has been held on 14<sup>th</sup> October 2019 in Paris between our group, the national network on metallurgy (RNM) and representants from industry. The purpose of the meeting was to present the activities of our group, our possibilities to measure or obtain by calculation thermodynamic data and the interest of the use of such data. Also, the needs from the industry and the academic community were presented.

### 4.5 French-German workshop

For the first time a workshop was organized in order to bring together the German and French communities working on thermodynamics, kinetics and phase diagrams. The workshop was organized by J.-M. Joubert and H. Seiffert and was held in Thiais at the ICMPE 21<sup>st</sup> and 22<sup>nd</sup> November 2019. Fifty participants attended the meeting.

## **5. Upcoming events in 2020**

### 5.1 Summer school on thermodynamics

Following two previous editions in 2015 and 2017, a summer school on thermodynamics: 'Thermodynamic data: from acquisition to application' (in French) will be organized by our group. It will be held on the island of Porquerolles in the south of France from 5<sup>th</sup> to 9<sup>th</sup> October 2020.

Flyer: [https://www.thermatht.fr/wp-content/uploads/2020/03/Flyer-Ecole-GdR-Oct-2020\\_v4.pdf](https://www.thermatht.fr/wp-content/uploads/2020/03/Flyer-Ecole-GdR-Oct-2020_v4.pdf)

Inscription : <https://www.azur-colloque.fr/DR07/inscription/preinscription/257/fr>

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

Together with the 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...

## 6. List of the teams and members of the GdR TherMatHT

### Contact persons in bold

Laboratoire	Nom	Prénom	email	Website	Systems of interest
Calcul Thermodynamique – Orcet	<b>Dupin</b>	<b>Nathalie</b>	nathdupin@cthermo.fr	<a href="http://cthermo.fr/">http://cthermo.fr/</a>	
CEA Cadarache DEN/DEC/SA3C/LAMIR	Pointillon	Yves			
	Fiquet	Olivier			
	Carlot	Gaelle			
	Dumas	Jean-Christophe			
	Martin	Philippe			
	Martin	Guillaume			
	Palancher	Hervé			
CEA Cadarache DEN/DEC/SPUA/LMPC	Belin	Renaud			
	Lechelle	Jacques			
CEA Cadarache DEN/DEC/SPUA/LTEC	Audubert	Fabienne			
CEA Cadarache DEN/DTN/STRI/LMA	Journeau	Christophe			
	<b>Piluso</b>	<b>Pascal</b>			
CEA Marcoule DEN/DTCD/SECM/LDMC	Agullo	Julia			
	Regnier	Elise			metals and alloys, glasses
CEA Marcoule DEN/DTEC/SDTC/LEMA	Delahaye	Thibaud			
CEA Saclay DEN/DMN/SRMA/LA2M	<b>Toffolon-Masclat</b>	<b>Caroline</b>	caroline.toffolon@cea.fr	<a href="https://www.universite-paris-saclay.fr/fr/recherche/laboratoire/service-de-recherches-metallurgiques-appliquees-srma-0">https://www.universite-paris-saclay.fr/fr/recherche/laboratoire/service-de-recherches-metallurgiques-appliquees-srma-0</a>	
	Roubaud	J.			
	Guilbert	Thomas			
CEA Saclay DEN/DMN/SRMA/LTME	Braun	James			
CEA Saclay DEN/DPC/SCCME/LM2T	Alpettaz	Thierry			

	Bordier	Sébastien			
	Chatain	Sylvie			
	<b>Gossé</b>	<b>Stéphane</b>	stephane.gosse@cea.fr		
	Guéneau	Christine			
	Lizon a Lugin	Eric			
	Quaini	Andrea			
CEA Saclay DEN/DPC/SCCME/LM2C	Freyss	Michel			UO2, PuO2, UPuO2, AmO2, UPuAmO2, CeO2, UCeO2
CEA Saclay DSM/IRAMIS/SI2SM/LEEL	Berger	Pascal			
	Khodja	Hicham			
	Raepsaet	Caroline			
CEA DTBH	Defoort	Françoise			
	Froment	Karine			
	Ravel	Serge			
	Seiler	Jean-Marie			
CEA Marcoule DEN/DTCD/SECM/LCLT	Nicoleau	Elodie			
CEA Marcoule DEN/DTCD/SECM/LDMC	Boué	Elodie			
	Cozzika	Théodore			
	Hugon	Isabelle			
	Laplace	Annabelle			
	Pinet	Olivier			
	<b>Schuller</b>	<b>Sophie</b>	sophie.schuller@cea.fr		
CEA Valduc	Oudot	Benoît	benoit.oudot@cea.fr	<a href="http://www.cea.fr/pages/le-cea/les-centres-cea/valduc.aspx">http://www.cea.fr/pages/le-cea/les-centres- cea/valduc.aspx</a>	actinides
CEMEF	<b>Gandin</b>	<b>Charles- André</b>	charles-Andre.gandin@mines- paristech.fr	<a href="https://www.cemef.mines-paristech.fr/">https://www.cemef.mines-paristech.fr/</a>	
	Guillemot	Gildas			
CEMHTI – Orléans	Bouchetou	Marie-Laure			
	<b>de Bilbao</b>	<b>Emmanuel</b>	emmanuel.debilbao@univ- orleans.fr	<a href="http://www.cemhti.cnrs-orleans.fr/">http://www.cemhti.cnrs-orleans.fr/</a>	
	Poirier	Jacques			
CIRIMAT – Toulouse	Blanc	Christine			
	Connetable	Damien			
	<b>Drouet</b>	<b>Christophe</b>	christophe.drouet@ensiacet.fr	<a href="http://www.cirimat.cnrs.fr/">http://www.cirimat.cnrs.fr/</a>	
	Lacaze	Jacques			
	Monceau	Daniel			Ti-O, Ti-O-N, Ti-Al-Zr-Sn-Mo-V-O-N-H, Ni-Al- Pt-Cr, Ni-O-C-H-N-S
	Rouaix Vande Put	Aurélie			
	Vahlas	Constantin			

	Barnabé	Antoine			Cu-Fe-O, Cu-Cr-O
CMTC – Grenoble	<b>Fischer</b>	<b>Evelyne</b>	Evelyne.Fischer@simap.grenoble-inp.fr	<a href="http://cmtc.grenoble-inp.fr/">http://cmtc.grenoble-inp.fr/</a>	
ICAMS – Bochum (Germany)	<b>Fries</b>	<b>Suzana</b>	suzana.g.fries@ruhr-uni-bochum.de	<a href="http://www.icams.de/content/">http://www.icams.de/content/</a>	
	Palumbo	Mauro			
ICB – Dijon	Barras	Florence			
	Bernard	Frédéric			
	<b>Dereux</b>	<b>Alain</b>	alain.dereux@u-bourgogne.fr	<a href="https://scanr.enseignementsup-recherche.gouv.fr/structure/201220440V">https://scanr.enseignementsup-recherche.gouv.fr/structure/201220440V</a>	
	Le Gallet	Sophie			
ICG – Montpellier	Berche	Alexandre			
	Tedenac	Jean-Claude			
	Jund	Philippe	pjund@univ-montp2.fr	<a href="https://www.umontpellier.fr/recherche/unites-de-recherche/institut-charles-gerhardt-montpellier-icgm">https://www.umontpellier.fr/recherche/unites-de-recherche/institut-charles-gerhardt-montpellier-icgm</a>	
ICMCB – Bordeaux	<b>Gorsse</b>	<b>Stéphane</b>	gorsse@icmcb-bordeaux.cnrs.fr	<a href="http://www.icmcb-bordeaux.cnrs.fr/">http://www.icmcb-bordeaux.cnrs.fr/</a>	HEA, CCA, RHEA, RCCA
IEMN – Lille	Hourlier	Jamila		<a href="https://www.iemn.fr/cellule-technologique-renatech">https://www.iemn.fr/cellule-technologique-renatech</a>	
	Wallart	Xavier			
IJL – Nancy	Aeby-Gautier	Elisabeth			
	Aranda	Lionel			
	Berthod	Patrice			
	Combeau	Hervé			
	Daloz	Dominique			
	David	Nicolas			
	Dehmas	Moukrane			
	Denis	Sabine			
	<b>Fiorani</b>	<b>Jean-Marc</b>	Jean-Marc.Fiorani@univ-lorraine.fr	<a href="https://ijl.univ-lorraine.fr/a-la-une/">https://ijl.univ-lorraine.fr/a-la-une/</a>	
	Geandier	Guillaume			
	Mathieu	Stéphane			
	Redjaimia	Abdelkrim			
	Teixeira	Julien			
	<b>Vilasi</b>	<b>Michel</b>	Michel.Vilasi@univ-lorraine.fr		
	Zaloznik	Miha			
	<b>Zollinger</b>	<b>Julien</b>	julien.zollinger@univ-lorraine.fr		
IM2NP – Marseille	<b>Benigni</b>	<b>Pierre</b>	p.benigni@univ-amu.fr	<a href="https://www.im2np.fr/fr/accueil">https://www.im2np.fr/fr/accueil</a>	Ag-Cd-In-Zr, Ag-Al, Al-B-C, Al-Zr, Cr-Te, Na <sub>2</sub> O-SiO <sub>2</sub> , Al-Mg-B-C, Cs-Mo-O, O-Pu-U, Cr-Cu-O, glasses
	Coulet	Marie-Vanessa			
	Favotto	Claude			

	Hassam	Sheherazade			
	Maugis	Philippe			Fe-C
	Mikaelian	Georges			Ag-Cd-In-Zr, Cr-Te
	Record	Marie-Christine			
	Rogez	Jacques			
ICMPE – Thiais	Crivello	Jean-Claude			DFT, phonon, machine learning
	<b>Joubert</b>	<b>Jean-Marc</b>	joubert@icmpe.cnrs.fr	<a href="http://www.icmpe.cnrs.fr/">http://www.icmpe.cnrs.fr/</a>	Mo-Ni, Mo-Ni-Re, Os-Pt, H-Mg, Cr-H, H-Hf, H-Zr, H-Nb, H-Nb-Zr, Mo-Ru, Mo-Ru-Tc, Al-Fe-V, Al-W, Ti-W, Al-Ti-W, Co-Cr-Fe-Mn-Ni, Al-Co-Cr-Fe-Ni-Ti, Cr-Fe-Nb-Sn-Zr, H-O-Zr, Cr-Fe-H-Nb-O-Sn-Zr
IPGP – Paris	Gaillardet	Jérôme			
	<b>Neuville</b>	<b>Daniel</b>	neuville@ipgp.fr	<a href="http://www.ipgp.fr/fr">http://www.ipgp.fr/fr</a>	
	Richet	Pascal			
	Roux	Jacques			
IRSN – Cadarache	Barrachin	Marc	marc.barrachin@irsn.fr	<a href="https://www.irsn.fr/FR/Pages/Home.aspx">https://www.irsn.fr/FR/Pages/Home.aspx</a>	
	Michel	B.			
	Piar	B.			
Lafarge LCR – St Quentin Fallavier				<a href="https://www.tenerrdis.fr/fr/annuaire/lafarge-centre-de-recherche/">https://www.tenerrdis.fr/fr/annuaire/lafarge-centre-de-recherche/</a>	
LCTS – Bordeaux	Jacques	Sylvain			
	Lepetitcorps	Yann			
	Mouret	Thibault			
	Rebillat	Francis			
	Roger	Jérôme			Si-C, Ti-Al-Si-C, Ti-Si-N-O
	<b>Teyssandier</b>	<b>Francis</b>	fteyssa@univ-perp.fr		
	Chahhou	Bilal			AICCr2, AICTi2, C2SiTi3
LGC – Toulouse	Cassayre	Laurent	laurent.cassayre@ensiacet.fr	<a href="https://lgc.cnrs.fr/">https://lgc.cnrs.fr/</a>	Cu-Fe-O, Cr-Fe-O, Co-Fe-O, Mn-Fe-O, C-H-O-N+inorganics
	Chamelot	Pierre			
LMGP – Grenoble				<a href="http://www.lmgp.grenoble-inp.fr/">http://www.lmgp.grenoble-inp.fr/</a>	
LMI – Lyon	Andrieux	Jérôme			Al-B-C, Co-Ni-W, Fe-Ni-W
	Auvray	Laurent			
	Carole	Davy			
	Cauwet	François			
	<b>Dezellus</b>	<b>Olivier</b>	olivier.dezellus@univ-lyon1.fr	<a href="http://lmi.cnrs.fr/">http://lmi.cnrs.fr/</a>	Al-Si-Fe, Al-Si-Ti, Al-C-Mg, C-Ti, C-Ti-Fe, Ag-Cu-Ti, Al-C-Si-Ti
	Ferro	Gabriel			
	Gardiola	Bruno			
	Samer	Nassim			
	Soulière	Véronique			
LNE – Paris	<b>Razouk</b>	<b>Refat</b>		<a href="https://www.lne.fr/">https://www.lne.fr/</a>	metrology
LPSC – Grenoble	<b>Ghetta</b>	<b>Véronique</b>	Veronique.Ghetta@lpsc.in2p3.fr	<a href="http://lpsc.in2p3.fr/index.php/fr/">http://lpsc.in2p3.fr/index.php/fr/</a>	

Centre des Matériaux – Corbeil-Essones	<b>Bienvenu</b>	<b>Yves</b>	yves.bienvenu@ensmp.fr	<a href="http://www.mat.mines-paristech.fr/Accueil/">http://www.mat.mines-paristech.fr/Accueil/</a>	
ONERA – Chatillon	Perrut	Mikaël	mikael.perrut@onera.fr	<a href="https://www.onera.fr/fr">https://www.onera.fr/fr</a>	
	Gheno	Thomas			diffusion in alloys
PROMES – Odeillo-Font Romeu	Abanades	Stéphane			
	<b>Balat-Pichelin</b>	<b>Marianne</b>	Marianne.Balat@promes.cnrs.fr	<a href="https://www.promes.cnrs.fr/">https://www.promes.cnrs.fr/</a>	
	Charpentier	Ludovic			
Surface de Verre et Interface – Paris	<b>Burov</b>	<b>Ekaterina</b>	Ekaterina.Burov@saint-gobain.com	<a href="https://svi.cnrs.fr/spip/?page=sommaire&amp;lang=en">https://svi.cnrs.fr/spip/?page=sommaire&amp;lang=en</a>	silicate glasses Al <sub>2</sub> O <sub>3</sub> -CaO-Na <sub>2</sub> O-SiO <sub>2</sub>
SETARAM – Caluire-et-Cuire	André	Rémi	andre@setaram.com	<a href="https://www.setaram.fr/">https://www.setaram.fr/</a>	
SIMaP – Grenoble	<b>Antoni</b>	<b>Annie</b>	aantoni@phelma.grenoble-inp.fr	<a href="http://simap.grenoble-inp.fr/">http://simap.grenoble-inp.fr/</a>	Al-Nb, Co-Fe-W, Fe-Mo-W, B-Fe-Ti, Mn-Al-C-Fe-Mn, Al-Cu-X
	Blanquet	Elisabeth			
	Chatillon	Christian			
	Chaussende	Didier			
	Duffar	Thierry			
	Hodaj	Fiqiri			
	Jakse	Noel			
	<b>Nuta</b>	<b>Ioana</b>	ioana.nuta@simap.grenoble-inp.fr		
	Pasturel	Alain			
	Tassin	Catherine			
	Etay	Jacqueline			
	<b>Pisch</b>	<b>Alexander</b>	alexander.pisch@simap.grenoble-inp.fr		CaO-K <sub>2</sub> O-SiO <sub>2</sub> , CaO-Al <sub>2</sub> O <sub>3</sub> -SiO <sub>2</sub> , CaO-Al <sub>2</sub> O <sub>3</sub> -TiO <sub>x</sub>
SPCTS – Limoges	Maître	Alexandre			
	<b>Rapaud</b>	<b>Olivier</b>	olivier.rapaud@unilim.fr	<a href="https://www.ircer.fr/">https://www.ircer.fr/</a>	B-C-Fe, B-C-Hf-O-Si, B-C-O-Si-Zr, High Entropy Ceramics, MAX phases, MXenes
	Rejasse	Florian			
	Trolliard	Gilles			
SYMME – Annecy	Antion	Caroline			
	Janghorban	Amin			
	<b>Lomello-Tafin</b>	<b>Marc</b>	marc.lomello@univ-savoie.fr	<a href="http://www.symme.univ-smb.fr/">http://www.symme.univ-smb.fr/</a>	
Thermodata	Cheyne	Bertrand			
UCCS – Lille	<b>Montagne</b>	<b>Lionel</b>	lionel.montagne@univ-lille1.fr	<a href="http://uccs.univ-lille1.fr/index.php/fr/">http://uccs.univ-lille1.fr/index.php/fr/</a>	
UMET – Lille	<b>Legris</b>	<b>Alexandre</b>	alexandre.legris@univ-lille1.fr	<a href="http://umet.univ-lille1.fr/">http://umet.univ-lille1.fr/</a>	
	Reumont	Guy			
ISCR – Rennes	Tougait	Olivier		<a href="https://iscr.univ-rennes1.fr/umr/">https://iscr.univ-rennes1.fr/umr/</a>	
Friedrich Alexander Universität – Erlangen-Nürnberg (Germany)	<b>de Ligny</b>	<b>Dominique</b>	dominique.de.ligny@fau.de	<a href="https://www.fau.de/">https://www.fau.de/</a>	



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

