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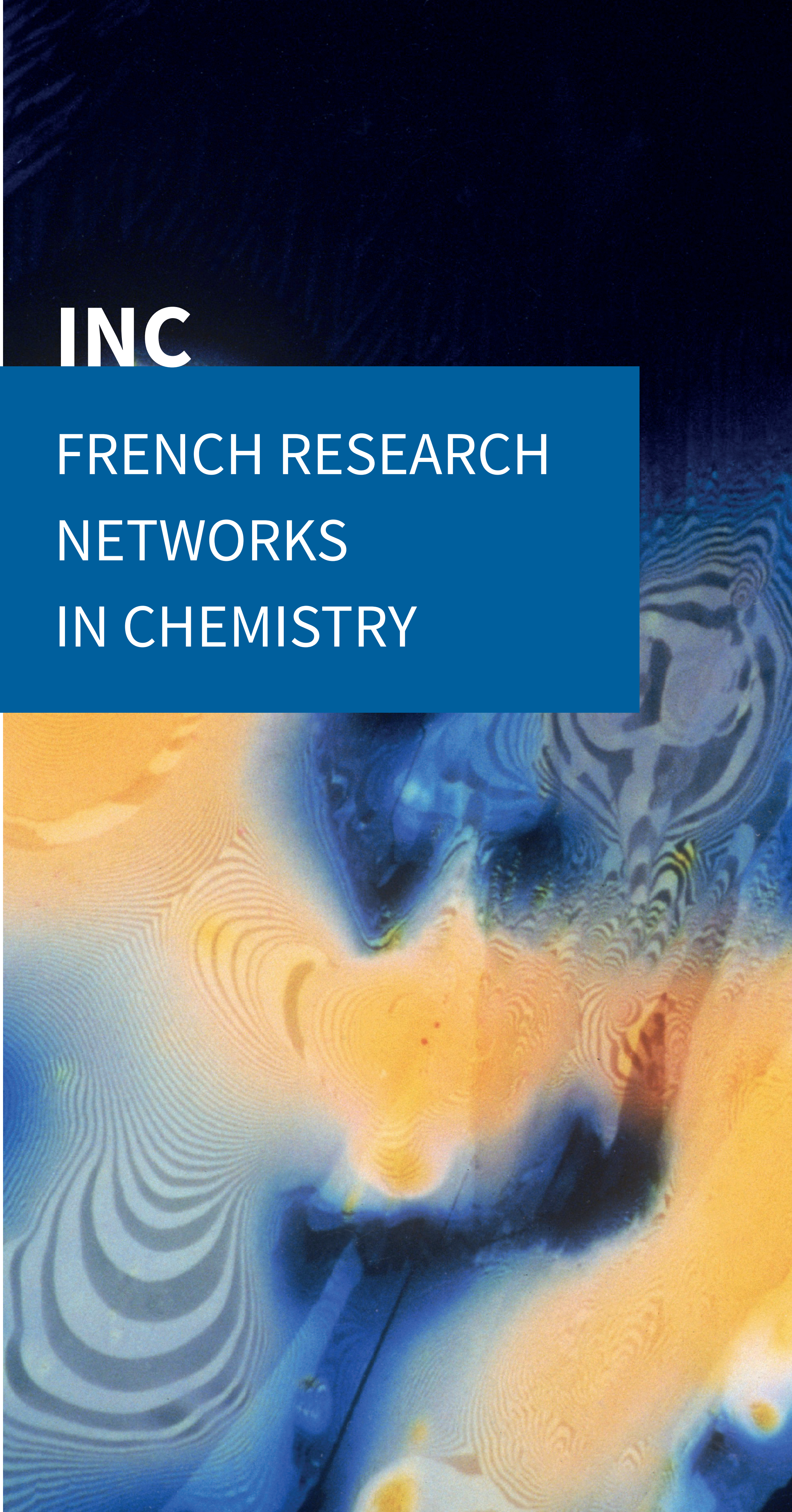
FRENCH RESEARCH NETWORKS IN CHEMISTRY

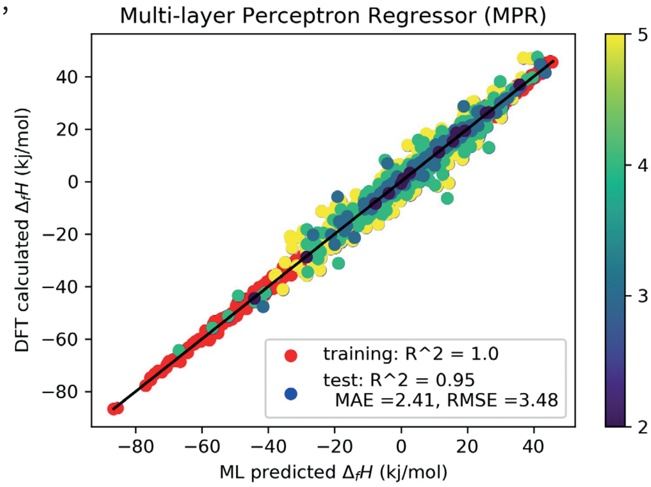


GDR THERMATHT

Materials thermodynamics at high temperature

OBJECTIVES

GDR THERMATHT was initially created with the objective of bringing together, federating and structuring the French community active in the field of thermodynamic data acquisition. The GDR scope goes actually far beyond data acquisition, opening itself to *ab-initio* calculations, Calphad modeling and more broadly to modeling of materials as well as their synthesis and transformation processes. The GDR also aims at promoting the discipline of thermodynamics, which involves the organization of 3 thematic schools and short training courses, through actions to open up to other communities in France (metallurgy, GDR Glass, etc.) and to abroad (DFG, APDIC, ThermoCon in the USA).



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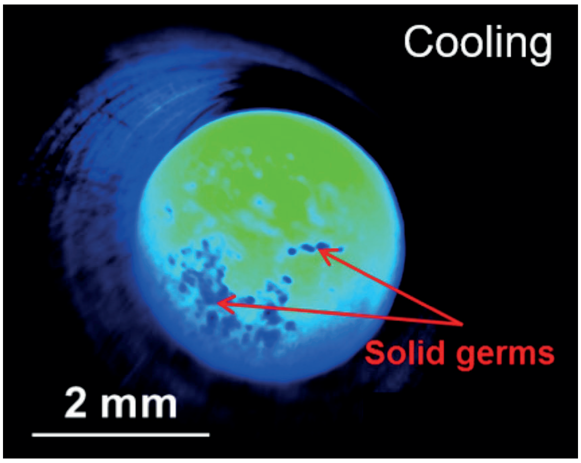
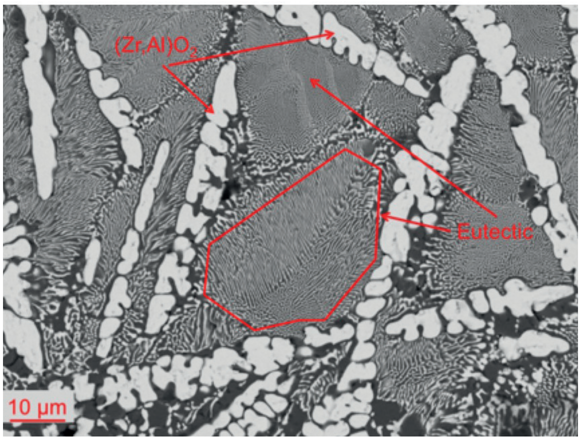
Coupling DFT calculations and machine learning to predict enthalpy of formation.





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Liquid Al_2O_3-ZrO_2 drop in levitation and its final microstructure. ATTILHA installation at CEA-Saclay.

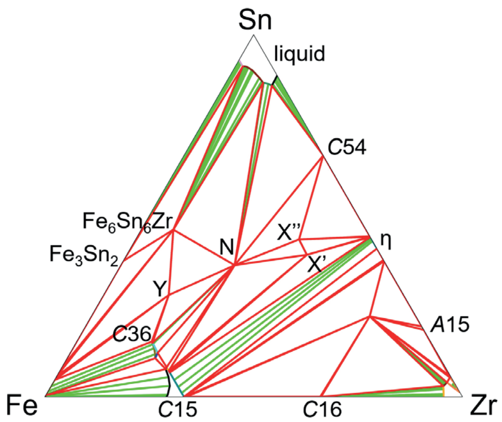
THEMATICS

- Thermodynamics of glasses
- Ultra high temperature measurements
- Calculations
- Metallurgy
- Silicon carbide

160 RESEARCHERS INVOLVED IN 40 LABORATORIES

PROSPECTS

For several years now, we have seen the emergence of digital techniques in materials science, with of course modeling which is becoming more and more quantitative at all scales, the design of alloys but also the advent of artificial intelligence that supports the development of new materials. These three directions highlight the critical need for reliable energy data and models on which calculation can be based.



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Isothermal section of Fe-Sn-Zr system @ 900°C.

The acquisition of thermodynamic data, through experience or *ab-initio* calculation, will therefore remain an important topic for decades to come. Much remains to be done, especially on refractory and ultra-refractory materials for which measurements are difficult but essential in many respects. One could cite as an example calcium aluminate which is a key compound in earth science and planetology as well as for industrial applications such as aluminous and Portland cements. Their thermodynamic properties at very high temperature (T> 2000K) are not well known and uncertainties exceeding 40% are frequently observed. Taking into account minor or trace elements in metal alloys, hitherto largely neglected, is becoming increasingly important with the aim of always better controlling and optimizing properties.

Historically, the Calphad method was developed on the basis of simple parametric energy models of practical interest but not representative of physics. The current trend is towards the development of so-called third-generation thermodynamic bases whose energy models are more firmly anchored in physics. It is for example important that heat capacities be compatible with the model of Einstein or to determine a model allowing an adequate and continuous description of the vitreous solids, between liquid and the crystal.

The perimeter of GDR THERMATHT was that of the bulk thermodynamic properties of phases. Interactions with other communities have highlighted a lack and therefore a need to make an effort on other thermodynamic quantities such as interfacial quantities or those associated with diffusion. Here again, process modeling requires the use of these quantities and therefore an effort in terms of measurement, understanding and modeling.

CONTACT

Director
Olivier Dezellus (LMI Lyon)
olivier.dezellus@univ-lyon1.fr

http://www.thermatht.fr

cnrs GDR Groupement de recherche
THERMATHT Material thermodynamics at high temperature