



APDIC report 2017

French contribution

Jean-Marc Joubert

22nd May 2018

1. Subscription of the GdR TherMatHT to the APDIC

Following the presentation made by Jean-Marc Joubert at the APDIC meeting in Saint-Malo (10th June 2017), the formal subscription of the GdR TherMatHT was approved in replacement of the former Groupe de Thermodynamique et Diagrammes de Phases. From now, it will be the French representative to the APDIC. Jean-Marc Joubert has been appointed to represent the GdR TherMatHT to the APDIC meetings.

GdR TherMatHT (<https://www.thermatht.fr/>) 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.

2. Main events related to Phase Diagrams

2.1. Organization of the Calphad conference

The Calphad XLVI meeting took place in Saint-Malo, a beautiful medieval city on the northern coast of French Brittany in the western France from June 11 to June 16, 2017. The conference was organized by Jean-Marc Joubert (ICMPE, Thiais) and Annie Antoni-Zdziobek (SIMAP, Grenoble). The first Calphad conference was organized by Larry Kaufman and H. Nesor in Cambridge, Massachusetts, USA, in November 1973, the previous meeting held in France was Calphad XXVIII, organized in Grenoble by Himo Ansara in 1999, and the last meeting was in Japan, organized by Tetsuo Mohri in 2016. Calphad XLVI attracted a high number of participants: 226 registered person (205 scientific attendees and 21 accompanying guests), from 26 countries.

The final scientific program included 6 keynote lectures, 79 oral presentations, 122 poster presentations organized into two different poster sessions (chair: M. Perrut), and 3 software demonstrations (Thermo-Calc, Pandat, and Fact-Sage, chair: Alexander Pisch). Oral presentations

were grouped into 10 different topics: Configurational thermodynamics, First-principles calculations, Thermo-kinetics and diffusion, Phase field and molecular dynamics, Interface and thin films, Thermodynamic assessments, Experimental measurements, Liquids and salts, New models, Applications.

A Young Calphadian Meeting took place on Monday evening (chair: S. Gossé) with informal presentations and discussions between experienced (B. Sundman, C. Colinet, B.-J. Lee) and younger Calphadians.

During the banquet several awards were announced including:

- the APDIC Best Paper Award, selected by APDIC among papers about phase diagrams and related topics published in 2016. It was attributed to Y. Dahan, G. Makov and R. Z. Shneck for the paper "Nanometric size dependent phase diagram of Bi-Sn", published in Calphad, 53, 2016, 136-145.
- the APDIC industrial award 2017, in recognition of the "Excellence in operational research, achievements in material dominated technologies or management, relating to Materials Chemistry and Phase Diagrams". It was given to Tenaris R&D Campana, Argentina.

<https://calphad2017.sciencesconf.org/>

2.2. Third edition of the SATA school

The third edition of the SATA school (School for Advanced Thermodynamic Assessments) was organized by Bo Sundman and Christine Guéneau at the Presqu'île de Giens, 3-7 July, 2017. The aim of the school is to provide an advanced course on thermodynamic modelling using the Calphad method. A central part of the school was the practical assessment of model parameters of multi-component systems for the development of thermodynamic databases.

The school gathered 12 students from around the world.

2.3. Annual meeting of the GdR TherMatHT

The Annual meeting of the GdR TherMatHT was held in Limoges January 26-27, 2017.

<https://thermatht4.sciencesconf.org/>

2.4. Subscription to ThermoCon

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/>

3. Upcoming events

3.1. Thermec

The International Conference on PROCESSING & MANUFACTURING OF ADVANCED MATERIALS, Processing, Fabrication, Properties, Applications (Thermec) will be held in Paris, July 8-13, 2018

<https://thermec2018.sciencesconf.org/>

3.2. Thermo-Calc user group meeting

Thermo-Calc will organize its French Computational and Kinetics Seminar in Nice on October 30, 2018.

3.2. Matériaux 2018

The largest French conference on materials, held every 4 years, will be organized in Strasbourg, November 19-23, 2018.

<http://www.materiaux2018.fr/>

4. List of the teams and members of the GdR TherMatHT

Laboratoire	Nom	Prénom
Calcul Thermodynamique	Dupin	Nathalie
CEA Cadarache DEN/DEC/SA3C/LAMIR	Pointillon	Yves
	Fiquet	Olivier
	Carlot	Gaëlle
	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
	Piluso	Pascal
CEA Marcoule DEN/DTCD/SECM/LDMC	Regnier	Elise
CEA Marcoule DEN/DTEC/SDTC/LEMA	Delahaye	Thibaud
CEA Saclay DEN/DMN/SRMA/LA2M	Toffolon-Masclat	Caroline
	Roubaud	J.
	Guilbert	T.
CEA Saclay DEN/DMN/SRMA/LTME	Braun	James
CEA Saclay DEN/DPC/SCCME/LM2T	Alpettaz	Thierry
	Bordier	Sébastien
	Chatain	Sylvie
	Gossé	Stéphane
	Guéneau	Christine
	Lizon a Lugrin	Éric
	Quaini	Andrea
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
	Schuller	Sophie
CEMHTI	Bouchetou	Marie-Laure
	de Bilbao	Emmanuel
	Poirier	Jacques
CIRIMAT	Blanc	Christine
	Connetable	Damien
	Drouet	Christophe
	Lacaze	Jacques
	Rouaix Vande Put	Aurélie
	Vahlas	Constantin
CMTC	Fischer	Evelyne
ICAMS	Fries	Suzana
	Palumbo	Mauro
ICB UMR 6303 CNRS / UB	Barras	Florence
	Bernard	Frédéric
	Dereux	Alain
	Le Gallet	Sophie
ICG Montpellier	Berche	Alexandre
	Tedenac	Jean-Claude
ICMCB	Gorsse	Stéphane
IEMN	Hourlier	Jamila
	Wallart	Xavier
IJL	Aeby-Gautier	Elisabeth
	Aranda	Lionel
	Berthod	Patrice
	Combeau	Hervé
	Daloz	Dominique
	David	Nicolas
	Dehmas	Moukrane
	Denis	Sabine
	Fiorani	Jean-Marc
	Geandier	Guillaume
	Mathieu	Stéphane
	Redjaimia	Abdelkrim
	Teixeira	Julien
	Vilasi	Michel
	Zaloznik	Miha
	Zollinger	Julien
IM2NP	Benigni	Pierre
	Coulet	Marie-Vanessa
	Favotto	Claude
	Hassam	Sheherazade
	Maugis	Philippe
	Mikaelian	Georges
	Rogez	Jacques
Institut de Chimie et des Matériaux Paris-Est (UMR7182)	Crivello	Jean-Claude
	Joubert	Jean-Marc
IPGP	Gaillardet	Jérôme
	Neuville	Daniel
	Richet	Pascal
	Roux	Jacques
IRSN	Barrachin	Marc
	Michel	B.
	Piar	B.
Lafarge LCR	Pisch	Alexander

LCTS	Jacques	Sylvain
	Lepetitcorps	Yann
	Rebillat	Francis
	Roger	Jérôme
	Teyssandier	Francis
LGC	Cassayre	Laurent
	Chamelot	Pierre
LMGP	Chaussende	Didier
LMI	Andrieux	Jérôme
	Auvray	Laurent
	Carole	Davy
	Cauwet	François
	Dezellus	Olivier
	Ferro	Gabriel
	Gardiola	Bruno
	Samer	Nassim
	Soulière	Véronique
LPSC	Ghetta	Véronique
Centre des Matériaux	Bienvenu	Yves
PROMES	Abanades	Stéphane
	Balat-Pichelin	Marianne
	Charpentier	Ludovic
SIMaP	Antoni	Annie
	Blanquet	Elisabeth
	Chatillon	Christian
	Duffar	Thierry
	Hodaj	Figiri
	Jakse	Noel
	Nuta	Ioana
	Pasturel	Alain
	Tassin	Catherine
	Etay	Jacqueline
SPCTS	Maître	Alexandre
	Rapaud	Olivier
	Rejasse	Florian
	Trolliard	Gilles
SYMME	Antion	Caroline
	Janghorban	Amin
	Lomello-Tafin	Marc
Thermodata	Cheyne	Bertrand
UCCS	Montagne	Lionel
UMET	Legris	Alexandre
	Reumont	Guy
Univ Rennes	Tougait	Olivier
Universität Erlangen-Nürnberg	de Ligny	Dominique

5. List of publications

A list of publications related to phase diagrams is given. It is meant to describe the activity of France in the field of phase diagrams for the year 2017. It has been obtained using Web of Science with the following key: Topic='phase diagram', Address='France', Year='2017'. The initial result (467 publications) was sorted and only the publications which seem really related to phase diagram studies are given below. Note that the list is probably non-exhaustive and some of the listed papers are only slightly related to phase diagrams studies in the meaning of the APDIC.

1.

Absence of magnetic ordering and field-induced phase diagram in the gadolinium aluminum garnet

By: Florea, O.; Lhotel, E.; Jacobsen, H.; et al.

PHYSICAL REVIEW B Volume: 96 Issue: 22 Article Number: 220413 Published: DEC 26 2017

2.

Phase equilibria of phenolic compounds in water or ethanol

- By: Cesari, Laetitia; Namysl, Sylvain; Canabady-Rochelle, Laetitia; et al.
FLUID PHASE EQUILIBRIA Volume: 453 Pages: 58-66 Published: DEC 15 2017
3.
Navigating at Will on the Water Phase Diagram
By: Pipolo, S.; Salanne, M.; Ferlat, G.; et al.
PHYSICAL REVIEW LETTERS Volume: 119 Issue: 24 Article Number: 245701 Published: DEC 14 2017
4.
Nitrogen Transfer between Solid Phases in the System Mn-N Detected via in situ Neutron Diffraction
By: Widenmeyer, Marc; Hansen, Thomas C.; Leineweber, Andreas; et al.
ZEITSCHRIFT FUR ANORGANISCHE UND ALLGEMEINE CHEMIE Volume: 643 Issue: 23 Special Issue: SI Pages: 1929-1938 Published: DEC 13 2017
5.
Comprehensive phase diagram of two-dimensional space charge doped Bi₂Sr₂CaCu₂O_{8+x}
By: Sterpetti, Edoardo; Biscaras, Johan; Erb, Andreas; et al.
NATURE COMMUNICATIONS Volume: 8 Article Number: 2060 Published: DEC 12 2017
6.
Melting Curve and Liquid Structure of Nitrogen Probed by X-ray Diffraction to 120 GPa
By: Weck, Gunnar; Datchi, Frederic; Garbarino, Gaston; et al.
PHYSICAL REVIEW LETTERS Volume: 119 Issue: 23 Article Number: 235701 Published: DEC 4 2017
7.
Structural Transitions in Elemental Tin at Ultra High Pressures up to 230 GPa
By: Gavriluk, A. G.; Troyan, I. A.; Ivanova, A. G.; et al.
JETP LETTERS Volume: 106 Issue: 11 Pages: 733-738 Published: DEC 2017
8.
Thermodynamic modeling of the V-Si-B system
By: Araujo Pinto da Silva, Antonio Augusto; Chaia, Nabil; Ferreira, Flavio; et al.
CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY Volume: 59 Pages: 199-206 Published: DEC 2017
9.
Phase transitions of Cu_{3+x}Si observed by temperature-dependent x-ray powder diffraction
By: Correa, Cinthia Antunes; Poupon, Morgane; Kopecek, Jaromir; et al.
INTERMETALLICS Volume: 91 Pages: 129-139 Published: DEC 2017
10.
Vaporization and condensation in the Al₄C₃-SiC system
By: Le-Tran, Hoang-Long; Sarigiannidou, Eirini; Gelard, Isabelle; et al.
JOURNAL OF THE EUROPEAN CERAMIC SOCIETY Volume: 37 Issue: 15 Pages: 4475-4482 Published: DEC 2017
11.
Hydrogen absorption in 1 nm Pd clusters confined in MIL-101(Cr)
By: Malouche, Abdelmalek; Blanita, Gabriela; Dan Lupu; et al.
JOURNAL OF MATERIALS CHEMISTRY A Volume: 5 Issue: 44 Pages: 23043-23052 Published: NOV 28 2017
12.
Coincidence of magnetic and valence quantum critical points in CeRhIn₅ under pressure
By: Ren, Z.; Scheerer, G. W.; Aoki, D.; et al.
PHYSICAL REVIEW B Volume: 96 Issue: 18 Article Number: 184524 Published: NOV 28 2017
13.
Metallurgy of soft spheres with hard core: From BCC to Frank-Kasper phases
By: Pansu, Brigitte; Sadoc, Jean-Francois
EUROPEAN PHYSICAL JOURNAL E Volume: 40 Issue: 11 Article Number: 102 Published: NOV 24 2017
14.
Chemical equilibrium for the reactive system propionic acid plus ethanol plus ethyl propionate + water at 303.15 and 313.15 K
By: Toikka, Maria; Sadaeva, Anna; Samarov, Artemiy; et al.
FLUID PHASE EQUILIBRIA Volume: 451 Pages: 91-95 Published: NOV 15 2017
15.
Nitridation enhancement of TiSi₂ powders by addition of nickel
By: Roger, J.; Nouvian, L.; Le Petitcorps, Y.; et al.
JOURNAL OF ALLOYS AND COMPOUNDS Volume: 724 Pages: 249-257 Published: NOV 15 2017
16.
Hume-Rothery for HEA classification and self-organizing map for phases and properties prediction
By: Calvo-Dahlborg, M.; Brown, S. G. R.
JOURNAL OF ALLOYS AND COMPOUNDS Volume: 724 Pages: 353-364 Published: NOV 15 2017
17.
Synthesis, Structure, and Electrochemical Properties of LiFeV₂O₇
By: Benabed, Yasmine; Castro, Laurent; Penin, Nicolas; et al.

CHEMISTRY OF MATERIALS Volume: 29 Issue: 21 Pages: 9292-9299 Published: NOV 14 2017

18.
Phase equilibria in the ternary B-Ce-Cu system with a thermodynamic reassessment of the binary B-Ce system
By: Premovic, Milena; Du, Yong; Zhang, Fan; et al.
THERMOCHIMICA ACTA Volume: 657 Pages: 185-196 Published: NOV 10 2017

19.
Hydration Phase Diagram of Clay Particles from Molecular Simulations
By: Honorio, Tulio; Brochard, Laurent; Vandamme, Matthieu
LANGMUIR Volume: 33 Issue: 44 Pages: 12766-12776 Published: NOV 7 2017

20.
(Oxo)(Fluoro)-Aluminates in KF-Al₂O₃ System: Thermal Stability and Structural Correlation
By: Simko, Frantisek; Rakhmatullin, Aydar; Florian, Pierre; et al.
INORGANIC CHEMISTRY Volume: 56 Issue: 21 Pages: 13349-13359 Published: NOV 6 2017

21.
Solidification sequence of Ni-Si-Cr similar to 3wt% B brazing alloys
By: Siredey-Schwaller, N.; Hamel-Akre, J.; Peltier, L.; et al.
WELDING IN THE WORLD Volume: 61 Issue: 6 Pages: 1253-1265 Published: NOV 2017

22.
Thermodynamic characterization of lithium monosilicide (LiSi) by means of calorimetry and DFT-calculations
By: Taubert, Franziska; Schwalbe, Sebastian; Seidel, Juergen; et al.
INTERNATIONAL JOURNAL OF MATERIALS RESEARCH Volume: 108 Issue: 11 Pages: 942-958 Published: NOV 2017

23.
Thermodynamic assessment of the Na-O and Na-U-O systems: Margin to the safe operation of SFRs
By: Smith, A. L.; Gueneau, C.; Fleche, J. -L.; et al.
JOURNAL OF CHEMICAL THERMODYNAMICS Volume: 114 Special Issue: SI Pages: 93-115 Published: NOV 2017

24.
Improved microstructure and thermoelectric properties of higher manganese silicide processed by reactive spark plasma sintering
By: Vives, S.; Navone, C.; Gaudin, E.; et al.
JOURNAL OF MATERIALS SCIENCE Volume: 52 Issue: 21 Pages: 12826-12833 Published: NOV 2017

25.
Molecular Simulation of the Phase Diagram of Methane Hydrate: Free Energy Calculations, Direct Coexistence Method, and Hyperparallel Tempering
By: Jin, Dongliang; Coasne, Benoit
LANGMUIR Volume: 33 Issue: 42 Pages: 11217-11230 Published: OCT 24 2017

26.
Mechanosynthesis of bcc alloys from Fe_{50-y}/2Co_{50-y}/2Sn_y mixtures ($2 \leq y \leq 33$) and B2 ordering by annealing at modest temperatures
By: Costa, B. F. O.; Malaman, B.; Le Caer, G.; et al.
Conference: International Conference on the Applications of the Mossbauer Effect (ICAME) Location: Saint Petersburg, RUSSIA Date: SEP 03-08, 2017
HYPERFINE INTERACTIONS Volume: 238 Article Number: 76 Published: OCT 19 2017

27.
Ir-Re binary alloys under extreme conditions and their electrocatalytic activity in methanol oxidation
By: Yusenko, Kirill V.; Bykova, Elena; Bykov, Maxim; et al.
ACTA MATERIALIA Volume: 139 Pages: 236-243 Published: OCT 15 2017

28.
Reinvestigation of phase equilibria in TbCl₃-LiCl binary system
By: Danczak, A.; Salamon, B.; Kapala, J.; et al.
JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY Volume: 130 Issue: 1 Pages: 25-33 Published: OCT 2017

29.
A defect model for UO_{2+x} based on electrical conductivity and deviation from stoichiometry measurements
By: Garcia, Philippe; Pizzi, Elisabetta; Dorado, Boris; et al.
JOURNAL OF NUCLEAR MATERIALS Volume: 494 Pages: 461-472 Published: OCT 2017

30.
Phase separation in the half-Heusler thermoelectric materials (Hf,Ti,Zr) NiSn
By: Berche, A.; Tedenac, J. C.; Jund, P.
SCRIPTA MATERIALIA Volume: 139 Pages: 122-125 Published: OCT 2017

31.
Experimental investigation of the Y-Fe-Ga ternary phase diagram: Phase equilibria and new isothermal section at 800 degrees C
By: Nouri, K.; Jemmali, M.; Walha, S.; et al.
JOURNAL OF ALLOYS AND COMPOUNDS Volume: 719 Pages: 256-263 Published: SEP 30 2017

32.
Disorder-order phase transition at high pressure in ammonium fluoride

By: Bellin, Christophe; Mafety, Adrien; Narayana, Chandrabhas; et al.
PHYSICAL REVIEW B Volume: 96 Issue: 9 Article Number: 094110 Published: SEP 25 2017
33.
Magnetic order, hysteresis, and phase coexistence in magnetoelectric LiCoPO₄
By: Fogh, Ellen; Toft-Petersen, Rasmus; Ressouche, Eric; et al.
PHYSICAL REVIEW B Volume: 96 Issue: 10 Article Number: 104420 Published: SEP 15 2017
34.
Infrared probe of the gap evolution across the phase diagram of Ba_{1-x}K_xFe₂As₂
By: Xu, B.; Dai, Y. M.; Xiao, H.; et al.
PHYSICAL REVIEW B Volume: 96 Issue: 11 Article Number: 115125 Published: SEP 15 2017
35.
The Na_xMoO₂ Phase Diagram ($(1/2) \leq x < 1$): An Electrochemical Devil's Staircase
By: Vitoux, Laura; Guignard, Marie; Suchomel, Matthew R.; et al.
CHEMISTRY OF MATERIALS Volume: 29 Issue: 17 Pages: 7243-7254 Published: SEP 12 2017
36.
New phases of osmium carbide from evolutionary algorithm and ab initio computations
By: Fadda, Alessandro; Fadda, Giuseppe
MATERIALS RESEARCH EXPRESS Volume: 4 Issue: 9 Article Number: 096503 Published: SEP 2017
37.
Polymorphic phase transition and morphotropic phase boundary in Ba_{1-x}CaxTi_{1-y}ZryO₃ ceramics
By: Ben Abdesslem, M.; Aydi, S.; Aydi, A.; et al.
APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING Volume: 123 Issue: 9 Article Number: 583 Published: SEP 2017
38.
Phosphoric acid partition in aqueous two phase systems
By: Falcon-Millan, Guadalupe; Pilar Gonzalez-Munoz, M.; Durand, Alain; et al.
JOURNAL OF MOLECULAR LIQUIDS Volume: 241 Pages: 967-973 Published: SEP 2017
39.
Experimental and topological determination of the pressure temperature phase diagram of morniflumate, a pharmaceutical ingredient with anti-inflammatory properties
By: Barrio, M.; Tamarit, J. -Ll; Ceolin, R.; et al.
JOURNAL OF CHEMICAL THERMODYNAMICS Volume: 112 Pages: 308-313 Published: SEP 2017
40.
Phase equilibrium data and modeling of ethylic biodiesel, with application to a non-edible vegetable oil
By: Muhammad, Fahad; Oliveira, Mariana B.; Pignat, Patrice; et al.
FUEL Volume: 203 Pages: 633-641 Published: SEP 1 2017
41.
Droplets-based millifluidic for the rapid determination of biopolymers phase diagrams
By: Amine, Chloe; Boire, Adeline; Davy, Joelle; et al.
FOOD HYDROCOLLOIDS Volume: 70 Pages: 134-142 Published: SEP 2017
42.
Study of the ternary system Al-H-RE (RE = Er, La and Y) in liquid state
By: Prigent, Jocelyn; Joubert, Jean-Marc; Latroche, Michel
Conference: 15th International Symposium on Metal-Hydrogen Systems (MH) Location: Interlaken, SWITZERLAND Date: AUG 07-12, 2016
INTERNATIONAL JOURNAL OF HYDROGEN ENERGY Volume: 42 Issue: 35 Special Issue: SI Pages: 22348-22352 Published: AUG 31 2017
43.
Phase transitions and magnetic properties of LuFe₂O₄ under pressure
By: Markovich, V.; Fita, I.; Wisniewski, A.; et al.
PHYSICAL REVIEW B Volume: 96 Issue: 5 Article Number: 054416 Published: AUG 11 2017
44.
Experimental Investigation of the Isothermal Section at 800 degrees C of the Nd-Fe-Co Ternary System
By: Bouchaala, N.; Jemmali, M.; Nouri, K.; et al.
JOURNAL OF PHASE EQUILIBRIA AND DIFFUSION Volume: 38 Issue: 4 Pages: 561-567 Published: AUG 2017
45.
Experimental investigation and thermodynamic evaluation of the C-Hf-O ternary system
By: Rejasse, Florian; Rapaud, Olivier; Trolliard, Gilles; et al.
JOURNAL OF THE AMERICAN CERAMIC SOCIETY Volume: 100 Issue: 8 Pages: 3757-3770 Published: AUG 2017
46.
Systematic First-Principles Study of Binary Metal Hydrides
By: Bourgeois, Natacha; Crivello, Jean-Claude; Cenedese, Pierre; et al.
ACS COMBINATORIAL SCIENCE Volume: 19 Issue: 8 Pages: 513-523 Published: AUG 2017
47.
Crystal structures of eta''-Cu₃+xSi and eta'''-Cu₃+xSi

By: Correa, Cinthia Antunes; Perez, Olivier; Kopecek, Jaromir; et al.
ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE CRYSTAL ENGINEERING AND MATERIALS Volume: 73 Special Issue: SI
Pages: 767-774 Part: 4 Published: AUG 2017

48.
Nd₂Ni₂MgH₈ hydride: Synthesis, structure and magnetic properties
By: Maskova, Silvie; Chotard, Jean-Noel; Denys, Roman V.; et al.
INTERMETALLICS Volume: 87 Pages: 13-20 Published: AUG 2017

49.
Phase equilibria in the Nd-Mg-Co system at 300 and 500 degrees C, crystal structure and hydrogenation behavior of selected compounds
By: Shtender, V.; Zelinska, O. Ya.; Pavlyuk, V. V.; et al.
INTERMETALLICS Volume: 87 Pages: 61-69 Published: AUG 2017

50.
Insight into the Am-O Phase Equilibria: A Thermodynamic Study Coupling High-Temperature XRD and CALPHAD Modeling
By: Epifano, Enrica; Gueneau, Christine; Belin, Renaud C.; et al.
INORGANIC CHEMISTRY Volume: 56 Issue: 13 Pages: 7416-7432 Published: JUL 3 2017

51.
High-pressure phase transitions of alpha-quartz under nonhydrostatic dynamic conditions: A reconnaissance study at PETRA III
By: Carl, Eva-Regine; Mansfeld, Ulrich; Liermann, Hanns-Peter; et al.
METEORITICS & PLANETARY SCIENCE Volume: 52 Issue: 7 Pages: 1465-1474 Published: JUL 2017

52.
Identification of NpO_{2+x} in the binary Np-O system
By: Tayal, Akhil; Conradson, Steven D.; Baldinozzi, Gianguido; et al.
JOURNAL OF NUCLEAR MATERIALS Volume: 490 Pages: 279-287 Published: JUL 2017

53.
Phase diagram of multiferroic KCu₃As₂O₇(OD)(3)
By: Nilsen, Goran J.; Simonet, Virginie; Colin, Claire V.; et al.
PHYSICAL REVIEW B Volume: 95 Issue: 21 Article Number: 214415 Published: JUN 20 2017

54.
Pressure-temperature phase diagram of the dimorphism of the anti-inflammatory drug nimesulide
By: Barrio, M.; Huguet, J.; Robert, B.; et al.
INTERNATIONAL JOURNAL OF PHARMACEUTICS Volume: 525 Issue: 1 Pages: 54-59 Published: JUN 15 2017

55.
Effective site-energy model: A thermodynamic approach applied to size-mismatched alloys
By: Berthier, F.; Creuze, J.; Legrand, B.
PHYSICAL REVIEW B Volume: 95 Issue: 22 Article Number: 224102 Published: JUN 8 2017

56.
The Pressure-Temperature Phase Diagram of Metacetamol and Its Comparison to the Phase Diagram of Paracetamol
By: Barrio, Maria; Huguet, Judit; Rietveld, Ivo B.; et al.
JOURNAL OF PHARMACEUTICAL SCIENCES Volume: 106 Issue: 6 Pages: 1538-1544 Published: JUN 2017

57.
Influence of the temperature and composition on the crystal structure of the AgBiSe₂-AgBiS₂ system
By: Mitra, Sunanda; Berardan, David
CRYSTAL RESEARCH AND TECHNOLOGY Volume: 52 Issue: 6 Article Number: 1700075 Published: JUN 2017

58.
Thermodynamic modelling of the Cr-Nb-Sn system
By: Lafaye, Paul; Toffolon-Masclat, Caroline; Crivello, Jean-Claude; et al.
CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY Volume: 57 Pages: 37-45 Published: JUN 2017

59.
Hypoeutectic melting in the UO₂-x-Gd₂O₃ system
By: Journeau, Christophe; Fouquart, Pascal; Domenger, Renaud; et al.
JOURNAL OF NUCLEAR MATERIALS Volume: 488 Pages: 287-294 Published: MAY 2017

60.
Characterization of saturated solutions and establishment of "a(w)-phase diagram" of ternary aqueous inorganic-organic and organic-organic systems
By: Dupas-Langlet, Marina; Benali, Mohammed; Pezron, Isabelle; et al.
JOURNAL OF FOOD ENGINEERING Volume: 201 Pages: 42-48 Published: MAY 2017

61.
Complete phase diagram of rare-earth nickelates from first-principles
By: Varignon, Julien; Grisolia, Mathieu N.; Iniguez, Jorge; et al.
NPJ QUANTUM MATERIALS Volume: 2 Article Number: 21 Published: APR 19 2017

62.
Supercritical Flow Synthesis of Pt_{1-x}Ru_x Nanoparticles: Comparative Phase Diagram Study of Nanostructure versus Bulk

By: Bondesgaard, Martin; Mainakhel, Aref; Becker, Jacob; et al.
CHEMISTRY OF MATERIALS Volume: 29 Issue: 7 Pages: 3265-3273 Published: APR 11 2017

63.
High-pressure high-temperature stability of hcp-IrxOs_{1-x} (x=0.50 and 0.55) alloys
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