



26-30.03.2017  
KARPACZ, POLAND

# 47<sup>èmes</sup> Journées des Actinides



Programme  
and  
Abstracts

# 47<sup>èmes</sup> Journées des Actinides

26 – 30 March 2017, Karpacz, Poland

organized by

Institute of Low Temperature and Structure Research  
Polish Academy of Sciences, Wrocław, Poland

*Programme and abstracts*

## Scope

**The 47èmes Journées des Actinides will be held in Karpacz, Poland between 26 and 30 March 2017.** The conference is an European, traditional, open and informal forum of the actinide community, devoted to all aspects (fundamental and applied) related to physics and chemistry of the 5f elements, their alloys and compounds. Topics that will be covered in this annual meeting include, but are not limited to (i) strongly correlated systems, superconductivity, quantum criticality, (ii) inorganic and organometallic chemistry, (iii) materials and nanomaterials, (iv) theory and band structure, (v) nuclear fuel cycle, environment, actinide production, fission products, actinide handling and radiation protection, nuclear forensics etc.

This year the JdA conference will incorporate **the FINUG 2017 Workshop** (Fundamental Research of Uranium Germanides and related compounds), being a part of a bilateral French-Polish CNRS-PAN cooperation program for the years 2015-2017. A special session will consist of talks of selected researchers (not only from France and Poland) presenting recent development in synthesis, crystallographic and physical characterization, and theoretical description of novel uranium germanides and related compounds.

## International Advisory Committee

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## Local Organizing Committee

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Bożena Dobrowolska  
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Krzysztof Domieracki

# 47 JdA Programme

**SUNDAY, 26<sup>th</sup> March 2017**

**Arrival by shuttle bus**

17:00 – 19:00      **Registration**

19:00 – 22:00      **Welcome party**

## MONDAY, 27<sup>th</sup> March 2017

8:40 – 9:00 **Welcome address**

9:00 – 10:15 **Session I**

Chairperson: D. Kaczorowski

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- 9:00 – 9:25 R. Troć  
“A rattling effect in actinide cage-type structures”
- 9:25 – 9:50 A.V. Andreev, Y. Skourski, D.I. Gorbunov  
“Magnetostriction at metamagnetic transition in  $\text{UCo}_2\text{Si}_2$ ”
- 9:50 – 10:15 L. Martel, A. Hen, Y. Tokunaga, J.-C. Griveau, E. Colineau,  
N. Magnani, J. Somers, R. Caciuffo  
“Investigation of the  $\text{U}_{0.15}\text{Np}_{0.85}\text{O}_2$  mixed oxide”

10:15 – 10:45 **Coffee break**

10:45 – 12:25 **Session II**

Chairperson: K. Gofryk

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- 10:45 – 11:10 P. M. Oppeneer  
“The hidden order phase of  $\text{URu}_2\text{Si}_2$  – An update on the status of its current understanding”
- 11:10 – 11:35 Z. Gajek and K. Durczewski  
“Influence of localized electrons on physical properties of the series  $\text{UT}_2\text{Al}_{10}$  (T = Fe, Ru, Os) and  $\text{REIn}_3$ ”
- 11:35 – 12:00 L. Sandratskii  
“Dzyaloshinskii-Moriya interaction and local magnetic anisotropies in  $\text{U}_2\text{Pd}_2\text{In}$ : Ground state and metamagnetic transition”
- 12:00 – 12:25 A. L. Kozub, A. B. Shick, T. Klimczuk  
“Electronic structure and magnetic properties of  $\text{NpPt}_2\text{In}_7$ ”

13:00 – 14:00 **Lunch**

15:00 – 16:40 **Session III**

Chairperson: L. Havela

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- 15:00 – 15:25 M. Werwiński, A. Szajek  
“Occupation deficiency in layered structures of  $\text{UNi}_x\text{Sb}_2$  ( $0 \leq x \leq 1$ ) studied by density functional theory supercell calculations”
- 15:25 – 15:50 S.Sowa, N.T.H. Kim-Ngan, M. Krupska, M. Paukov, V. Buturlim, L.Havela  
“U alloyed with selected *d*-metals: Structure and superconductivity”
- 15:50 – 16:15 J.E. Sutcliffe, T. Cartwright, P. Ryan, T.B. Scott, R.S. Springell  
“The Isothermal Martensitic Transformation in Metastable Uranium Alloys”
- 16:15 – 16:40 S. Maskova, A. Hen, M. Gelbstein, I. Orion, I. Halevy  
“Superconductivity in High Entropy Alloys - attempts to find Uranium containing High Entropy Alloy”

16:40 – 17:10 **Coffee break**

17:10 – 18:50 **Session IV**

Chairperson: M. Pasturel

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- 17:10 – 17:35 V. Sladkov, A.A. Bessonov, A.M. Fedosseev, I.A. Charushnikova  
“Complexation of U(VI) and Pu(VI) with succinic acid in aqueous acid solutions”
- 17.35 – 18:00 M. Saab, F. Réal, M. Šulka, F. Viro, L. Cantrel, V. Vallet  
“Quantum chemical prediction of standard formation enthalpies of uranyl nitrates and its degradation products”
- 18:00 – 18:25 F. Calard, A. Charlot, A. Leydier, F. Cuer, A. Grandjean  
“Hybrid Mesoporous Silicas Design For Uranium Extraction From Sulfuric Media”
- 18:25 – 18:50 I. Izosimov  
“Laser Spectroscopy and Detection of Actinides/Lanthanides in Biological Samples”

19:00 – 20:00 **Dinner**

20:00 – 22:00 **Poster session**

## TUESDAY, 28<sup>th</sup> March 2017

9:00 – 10:15 **Session V**

Chairperson: L. Sandratskii

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- 9:00 – 9:25 B. Dorado, J. Bieder, M. Torrent  
“Full first-principles calculation of Pu self-diffusion coefficient in Pu-Ga”
- 9:25 – 9:50 D. Legut, U. D. Wdowik, P. Piekarczyk, G. Jaglo  
“Electron correlations and spin-orbit coupling for lattice dynamics of UC and UO<sub>2</sub>”
- 9:50 – 10:15 L. Andrea, P. Garcia, M. Torrent, B. Dorado  
“Ab-initio calculation of oxygen interstitialcy diffusion mechanism in uranium dioxide UO<sub>2</sub> with paramagnetic ordering”

10:15 – 10:45 **Coffee break**

10:45 – 12:25 **Session VI**

Chairperson: J. Grin

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- 10:45 – 11:10 A. Leithe-Jasper, R. Gumeniuk, J. Grin  
“New actinide-based intermetallic compounds”
- 11:10 – 11:35 A.P. Gonçalves, I.C. Santos, E.B. Lopes, L.C.J. Pereira, M.S. Henriques, N. Zahurakova, V. Kontul', M. Reiffers  
“U<sub>2</sub>Sb: a novel binary uranium antimonide”
- 11:35 – 12:00 K. Domieracki, D. Kaczorowski  
“Comparative study of superconductivity in non-centrosymmetric silicides ThTESi (TE = Co, Ni, Pt)”
- 12:00 – 12:25 D. Gnida, P. Swatek  
“Quantum interference in disordered Th<sub>2</sub>CoSi<sub>3</sub>”

13:00 – 14:00 **Lunch**

### EXCURSION OR FREE TIME

19:00 – 20:00 **Dinner**

20:00 – 22:00 **Structured discussion**

## WEDNESDAY, 29<sup>th</sup> March 2017

9:00 – 10:15 **Session VII**

Chairperson: B. Dorado

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- 9:00 – 9:25 J. Jung, M. Atanasov, F. Neese  
“Ab initio ligand field analysis and covalency trends in lanthanide and actinide free ions and octahedral complexes”
- 9:25 – 9:50 S. Kervazo, F. Réal, F. Virost, A. S. P. Gomes, M. Olejniczak, P. Ayers, V. Vallet  
”Relativistic correlated calculations of the thermodynamics properties of gaseous plutonium oxides”
- 9:50 – 10:15 S. T. Murphy, C. Degauldre  
“On the state of Xe,Kr nature in actinide oxides: a solid study”

10:15 – 10:45 **Coffee break**

10:45 – 12:25 **Session VIII**

Chairperson: A. Gonçalves

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- 10:45 – 11:10 L. Havela, M. Paukov, V. Buturlim, I. Tkach, D. Drozdenko, M. Cieslar, S. Mašková, M. Dopita, Z. Matěj  
“Electrical resistivity of nanocrystalline Uranium hydrides affected by static and dynamic disorder”
- 11:10 – 11:35 P. Höhn, A. Amon, M. Bobnar, W. Schnelle, Y. Grin  
“New ternary uranium nitrides”
- 11:35 – 12:00 S. Maskova, K. Miliyanchuk, L. Havela  
“Hydrogen absorption in  $U_3Si_2$  and its impact on electronic properties”
- 12:00 – 12:25 V. Buturlim, L. Havela, S. Sowa, N.T.H. Kim-Ngan, M. Paukov, D. Drozdenko, M. Dopita, P. Minarik, S. Mašková  
„Development of bcc phase in  $U_{1-x}Ti_x$  system ( $x = 0.05-0.50$ ) and magnetic properties of related hydrides“

13:00 – 14:00 **Lunch**

15:00 – 16:40 **Session IX FINUG**

Chairperson: A. Pikul

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15:00 – 15:40 K. Gofryk, M. Jaime, A. Saul, M. Salamon, V.S. Zapf, N. Harrison,  
T. Durakiewicz, J.C. Lashley, D.A. Andersson, C. Stanek, J.L. Smith  
“Unusual thermal behavior of uranium dioxide”

15:40 – 16:20 M. Pasturel, A. Pikul  
“Phase formation, crystallographic relations and physical properties in  
the U-T-Ge ternary systems (T = transition metal from columns 8 to  
11): a comparative review”

16:20 – 16:40 M. Szlawska, D. Gnida, M. Daszkiewicz, D. Kaczorowski  
“Magnetic ordering in single-crystalline URhGe<sub>2</sub>”

16:40 – 17:10 **Coffee break**

17:10 – 18:00 **Session X**

*conference picture*

Chairperson: I. Halevy

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17:10 – 17:35 E. Lawrence Bright, S. Rennie, J. Darnbrough, D. Goddard,  
R. Springell  
“Uranium Nitride Thin Films for Accident Tolerant Fuels Research”

17:35 – 18:00 A. Keatley, T. Scott, R. Awbery  
“An investigation into the heterogeneity of vein type uranium ore  
deposits: Implications for nuclear forensic analysis”

18:00 – 18:25 **Summary and prospects**

20:00 – 22:00 **Conference banquet**

**THURSDAY, 30<sup>th</sup> March 2017**

**Departure by shuttle bus**

## List of poster presentations

- POSTER-1** A.V. Andreev, S. Daniš, J. Šebek, M.S. Henriques, J. Vejpravová, D.I. Gorbunov, L. Havela  
“Crystal Structure and Magnetism of UOsAl”
- POSTER-2** A.V. Andreev, J. Šebek, K. Shirasaki, T. Yamamura, L. Havela  
“Magnetism of  $\text{UCo}_{1-x}\text{OsAl}$  at low (<2%) Os content – transition from itinerant metamagnet to ferromagnet”
- POSTER-3** G. Chajewski, N. Brisset, C. Moussa, A. P. Pikul, M. Pasturel, O. Tougait  
“Magnetoresistivity of  $\text{U}_3\text{TGe}_5$  compounds (T = Ti, V, Cr, Nb, Mo, W)”
- POSTER-4** S. Chowdhury, M.S. Henriques, L. Maria, A. Cruz, L.M.Ferreira, T. Stora, A.P. Gonçalves  
“Electrospinning, an efficient way to prepare  $\text{YC}_x$  at nanoscales?”
- POSTER-5** M. Falkowski  
“Thermal and electron transport properties of  $\text{Ce}_2\text{Ni}_3\text{Ge}_5$  and  $\text{Ce}_3\text{NiGe}_2$ ”
- POSTER-6** S. Fryars, M. Pasturel, A. Pikul  
“Novel phases and phase equilibria at 1000 K in the U-Cu-Ge ternary system”
- POSTER-7** R. M. Harker, J. E. Darnbrough, D. Wermeille, G. H. Lander and R. Springell  
“Evidence for H incorporation into  $\text{UO}_2$  overlayers through synchrotron X-ray radiation”
- POSTER-8** J. Jung, K. Meyer, M. Atanasov, F. Neese  
“Ab initio ligand field theory applied to  $\text{U}^{\text{III}}$  and  $\text{U}^{\text{V}}$  complexes”
- POSTER-9** T.K.Kopeć, V. Apinyan  
“Superfluidity in two dimensional excitonic systems”
- POSTER-10** J. Lennard, V. Varsani  
“A Novel Method to Homogenise  $\delta$ -Pu-Ga Alloys by Using High-Temperature Thermal-Cycling and Ce - 5.04 at% La as a Surrogate”
- POSTER-11** Z. Molcanova, M. Mihalik, M. Mihalik, M. Zentkova, M. Rajnak, M. Hurakova, A. Dzubinska, M. Reiffers, M. Paukov, L. Havela, M. Cieslar, K. Milianchuk  
“Comparison of structural and magnetic properties of  $\text{UNiX}_2$  (X= Si, Ge) prepared by conventional method and splat cooling”

**POSTER-12** D.W. Wheeler, S.M. Ennaceur, M.B. Matthews, P. Roussel, P.D. Bayer  
“Observation and characterisation of a Pu-0.55 wt. % Ga alloy”

**POSTER-13** D.W. Wheeler  
“The use of nanoindentation to study the mechanical properties of cerium-lanthanum alloys”

**POSTER-14** D.W. Wheeler  
“A kinetic and mechanistic study of the oxidation of a cerium – 5 wt.% lanthanum alloy”

sun 26/03		mon 27/03		tue 28/03		wed 29/03		thu 30/03	
7:30 – 8:40	shuttle bus arrival	breakfast	excursion	breakfast	FINUG session (Gofryk, Pasturel, Szlawaska)	breakfast	shuttle bus departure	breakfast	
8:40 – 9:00		welcome address		Dorado		Jung			
9:00 – 9:25		Troć		Legut		Kervazo			
9:25 – 9:50		Andreev		Andrea		Murphy			
9:50 – 10:15		Colineau		coffee break		coffee break			
10:15 – 10:45		coffee break		Leithe-Jasper		Havela			
10:45 – 11:10		Oppeneer		Gonçalves		Höhn			
11:10 – 11:35		Gajek		Domieracki		Maškova			
11:35 – 12:00		Sandratskii		Gnida		Buturlim			
12:00 – 12:25		Kozub		lunch		lunch			
13:00 – 14:00		lunch							
15:00 – 15:25		Werwiński							
15:25 – 15:50		Sowa							
15:50 – 16:15		Sutcliffe							
16:15 – 16:40		Halevy							
16:40 – 17:10	coffee break								
17:10 – 17:35	Sladkov								
17:35 – 18:00	Saab								
18:00 – 18:25	Calard								
18:25 – 18:50	Izosimov								
19:00 – 20:00	dinner	dinner							
20:00 – 22:00	welcome party	posters	structured discussion	banquet					