

Programme & The Book of Abstracts

Nineteenth Annual Conference

YUCOMAT 2017

Herceg Novi, Montenegro, September 4-8, 2017

Organised by

MATERIALS RESEARCH SOCIETY OF SERBIA

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NINETEENTH ANNUAL CONFERENCE

YUCOMAT 2017

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,
September 4-8, 2017
<http://www.mrs-serbia.org.rs>

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Organised by:
Materials Research Society of Serbia

Endorsed by:
**Materials Research Society,
European Materials Research Society
and
Federation of European Material Societies**

Title: THE NINETEENTH ANNUAL CONFERENCE
YUCOMAT 2017
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Publisher: Materials Research Society of Serbia
Knez Mihailova 35/IV, P.O.Box 433, 11000 Belgrade, Serbia
Phone: +381 11 2185-437
<http://www.mrs-serbia.org.rs>

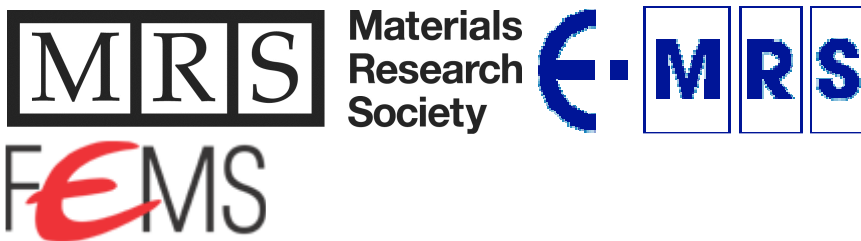
Editors: Prof. Dr. Dragan P. Uskoković and Prof. Dr. Velimir Radmilović

Technical editor: Aleksandra Stojičić

Cover page: Aleksandra Stojičić and Milica Ševkušić
Front cover: Modified Photo by Mercy; Wikimedia Commons
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Acknowledgments: This conference is celebrating 20 years of MRS-Serbia.



Printed in: Biro Konto
Sutorina bb, Igalo – Herceg Novi, Montenegro
Phones: +382-31-670123, 670025, E-mail: bkonto@t-com.me
Circulation: 220 copies. The end of printing: August 2017

P.S.B.10.

High-energy spectroscopy of YbM₂P₂ compounds

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We have studied experimentally and theoretically the electronic structure and x-ray absorption spectrum at the Yb L3 -edge and x-ray emission spectra of M and P at the K- and L_{2,3} -edges in the mixed valence compound YbM₂P₂ (with ThCr₂Si₂ type crystal structure), where M=Fe, Co, Ni. The theoretical calculations have been carried out by means of the ab initio fully-relativistic spin-polarized Dirac linear muffin-tin orbital method. The calculations show good agreement with the experimental measurements. The LSDA +U with $U_{\text{eff}} > 8.8$ eV produces two independent self-consistent solutions YbNi₂P₂ with divalent Yb²⁺ and trivalent Yb³⁺ ions. For the divalent Yb ion we found a non-magnetic solution with fourteen 4f electron bands completely occupied and situated far below the Fermi level. For trivalent Yb³⁺ solution thirteen 4f electron bands are situated well below the Fermi level. The hole 4f level for the Yb³⁺ solution the completely empty and situated sufficiently far from the Fermi level, therefore YbNi₂P₂ belong to the in homogeneously mixed-valence compounds. The calculated total magnetic moment for the Yb³⁺ solution moment is dominated by the 4f compounds, the spin Ms and orbital MI moments are 0.365 μ_B , and 1.135 μ_B , respectively. The spin and orbital moments at the Ni and P sites are very small: Ms Ni = - 0.0028 B, MsP = -0.0017 μ_B , MINi = -0.0019 μ_B and MIP = 0.0004 μ_B . Both the trivalent and the divalent Yb ions in are reflected in the experimentally measured Yb L3 x-ray absorption spectrum simultaneously. We found that the best agreement between the experimental spectrum and sum of the theoretically calculated Yb²⁺ and Yb³⁺ spectra is achieved with 73% ytterbium ions ²⁺ state and 27% ions in ³⁺ state. We found that the effect of the electronic quadrupole E2 transitions as well as the core-hole effect in the final states has minor influence on the intensity and the shape of the Ni and P K and L_{2,3} emission spectra as well as on the Yb L3 absorption spectrum. We would like to point out that the LSDA +U method which combines LSDA with a basically static, i.e. Hartree-Fock-like, mean -field approximation for a multi-band Anderson lattice model does not contain true many body physics. However, this method can be considered as the first step towards a better description of strongly correlated electron systems. The LSDA +U method provides the correct energy position of 4f energy bands and gives a reasonable description of the XAS and XES properties in YbNi₂P₂. However, the energy band structure for finite temperatures and the presumed Kondo lattice and mixed valence behavior in YbNi₂P₂ clearly requires a treatment that goes beyond a static mean-field approximation and includes dynamical effects, e.g., the frequency dependence of the self-energy.

CIP- Каталогизација у публикацији
Народна библиотека Србије

66.017/.018(048)

MATERIALS Research Society (Beograd). Conference (19 ; 2017 ; Herceg Novi)

Programme ; and The Book of Abstracts / Nineteenth Annual Conference YUCOMAT 2017, Herceg Novi, September 4-8, 2017 ; organised by Materials Research Society of Serbia, [Belgrade ; editors Dragan P. Uskoković and Velimir Radmilović]. - Belgrade : Materials Research Society of Serbia, 2017 (Herceg Novi : Biro Konto). - XL, 124 str. ; 23 cm

Tiraž 220. - Registar.

ISBN 978-86-919111-2-6

1. Materials Research Society of Serbia (Beograd)

- a) Наука о материјалима - Апстракти
- b) Технички материјали - Апстракти

COBISS.SR-ID 241612044