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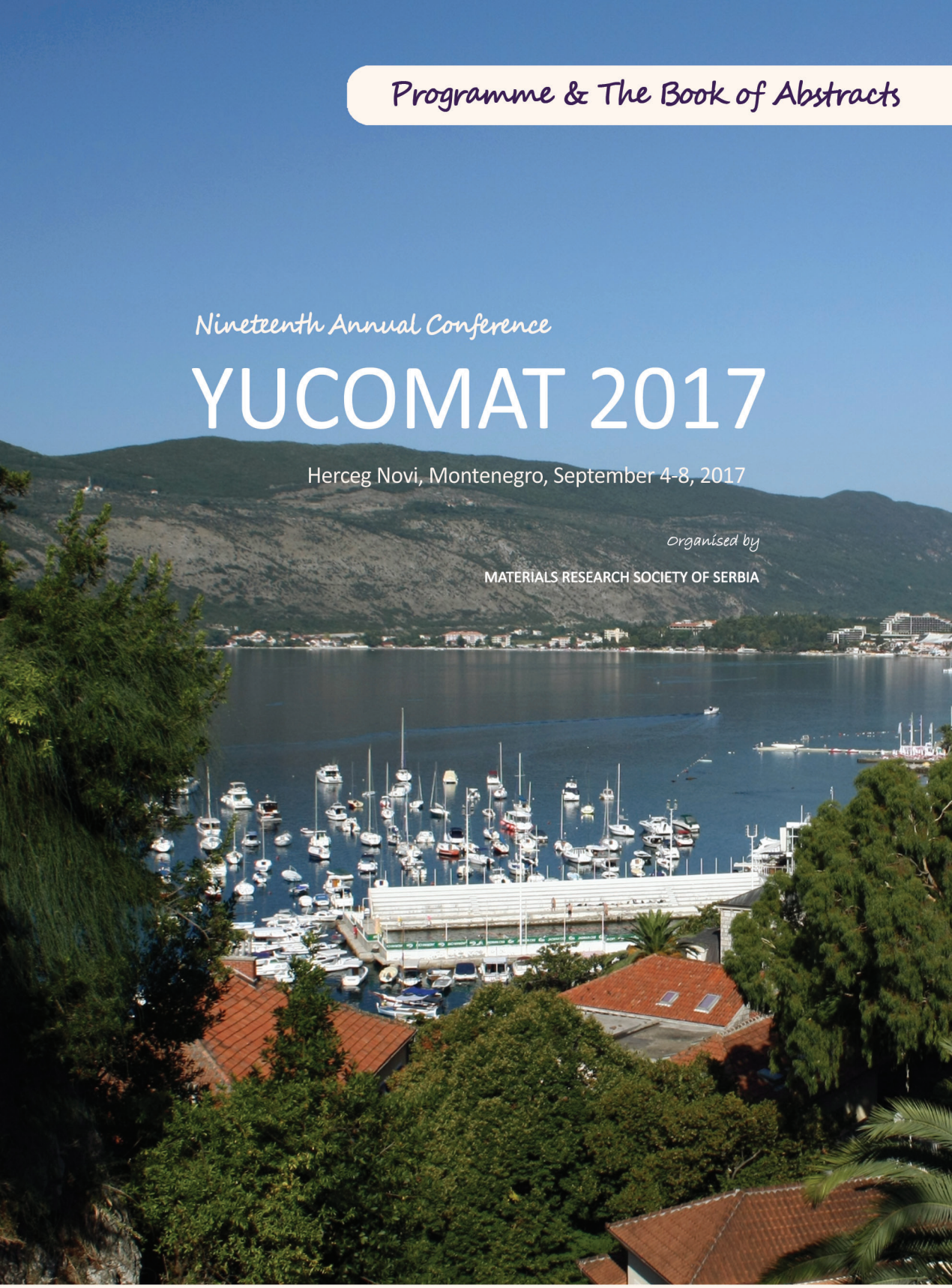

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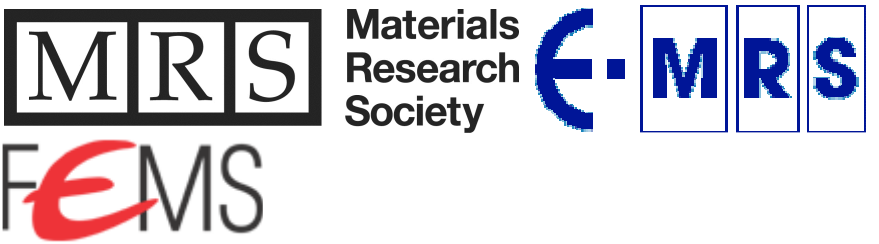

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High-energy spectroscopy of YbM_2P_2 compounds

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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 L2,3 -edges in the mixed valence compound YbM2P2 (with $ThCr_2Si_2$ 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 Ueff > 8.8 eV produces two independent self-consistent solutions $YbNi_2P_2$ with divalent Yb^{2+} and trivalent Yb^{3+} 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 Yb^{3+} solution thirteen 4f electron bands are situated well below the Fermi level. The hole 4f level for the Yb^{3+} solution the completely empty and situated sufficiently far from the Fermi level, therefore $YbNi_2P_2$ belong to the in homogeneously mixed-valence compounds. The calculated total magnetic moment for the Yb^{3+} solution moment is dominated by the 4f compounds, the spin Ms and orbital Ml moments are 0.365 μB, and 1.135 μB, respectively. The spin and orbital moments at the Ni and P sites are very small: Ms Ni= - 0.0028 B, MsP=-0.0017 μB, MlNi =-0.0019 μB and MlP =0.0004 μB. 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 Yb^{2+} and Yb^{3+} 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 L2.3 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 $YbNi_2P_2$. However, the energy band structure for finite temperatures and the presumed Kondo lattice and mixed valence behavior in $YbNi_2P_2$ clearly requires a treatment that goes beyond a static mean-field approximation and includes dynamical effects, e.g., the frequency dependence of the sell-energy.

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