SMARTER6

2. do 6. september 2018

predavalnica A, Fakulteta za kemijo in kemijsko tehnologijo, Ljubljana

ponedeljek, 3. september 2018

$9^{00} : 9^{50}$	S. Ashbrook (planarno predavanje): *Exploring the Hydration of the Inner Earth: Multinuclear NMR Spectroscopy and Ab Initio Random Structure Searching*
$9^{50} : 10^{10}$	L. Mafra: *New Insights into the Structure of Chemisorbed CO_2 Species in Mesoporous Solids Enabled by NMR and Computational Methods*
$10^{10} : 10^{30}$	Y. G. Kolyagin: *1D And 2D CPMG-based MAS NMR Methods for Zeolite Structure Elucidation: Tin Localization in Sn-BEA*
$10^{30} : 11^{00}$	odmor za kavo
$11^{00} : 11^{50}$	L. McCusker (planarno predavanje): *When X-Ray Powder Diffraction Is Not Enough*
$11^{50} : 12^{10}$	P. B. Groszewicz: *Tilting in Functional Perovskite Oxides: The Search for Structure-Property Relations Aided by Solid-State NMR*
$12^{10} : 12^{30}$	H. Geddes: *Compositional Inhomogeity in Mixed-Metal MOFs*
$12^{30} : 14^{00}$	kosilo
$14^{00} : 14^{20}$	S. Popović: *Contemporary Diffraction Methods in Study of Microstructure and Crystal Structure*
$14^{20} : 14^{40}$	J. Berryman: *Kinetic Control of Chiral Self Assembly: Selecting Mesoscopic Polymorphs Via Atomistic Information*
$14^{40} : 15^{00}$	sponzorsko predavanje
$15^{00} : 16^{00}$	poster sekcija
$16^{00} : 16^{20}$	E. Breynaert: *Solid-State MAS NMR and XRD Investigation of Cu Location in Cu-Loaded Zeolites*
$16^{20} : 16^{40}$	G. Szalontai: *ssNMR Spectroscopy, Crystallography and Computation Of Paramagnetic bis amino acid (κ^2N,O) copper(II) complexes. A Joint Approach.*
$16^{40} : 17^{00}$	Y. Nishiyama: *Understanding Hydrogen Bonding Structure by Electron and NMR Nano-Crystallography*

torek, 4. september 2018

$9^{00} : 9^{50}$	V. Blatov (planarno predavanje): *A Topological Model of Framework Assemblage for Predicting New Zeolites*
$9^{50} : 10^{10}$	S. P. Brown: *Using NMR Crystallography for Structural Elucidation and Insight*
$10^{10} : 10^{30}$	V. Diez-Gómez: *EFG Averaging Induced by Local Li Motion in NASICON Structures*

10^{30} : 11^{00} odmor za kavo

11^{00} : 11^{50} J. Reimer (planarno predavanje): *NMR and The Grand Challenges in MOF Research*

11^{50} : 12^{10} U. G. Nielsen: *Reliable Structural Characterization of Layered Double Hydroxides*

12^{10} : 12^{30} A. Hofstetter: *Predicting Chemical Shifts of Molecular Crystals by Machine Learning*

sreda, 5. september 2018

9^{00} : 9^{50} G. Dražić (planarno predavanje): *Direct Observation of Crystal Structure and Defects Using Cs Corrected Scanning Transmission Electron Microscopy*

9^{50} : 10^{10} Y. Khimyak: *Probing Organisation of "Crystalline" Gels Using NMR Spectroscopy: Gelation, Crystallisation and Dynamics of Self-Assembly*

10^{10} : 10^{30} G. Mollica: *Long-Range Carbon-Carbon J-couplings for NMR Crystallography of Small Organic Molecules*

10^{30} : 11^{00} odmor za kavo

11^{00} : 11^{50} M. Neumann (planarno predavanje): *How Many Ritonavir Cases Are Still Out There?*

11^{50} : 12^{10} W. Glossop: *Charactering Dynamics in Crystalline Solids Using MD Simulation and Solid-State NMR*

12^{10} : 12^{30} H. Boström: *Understanding Orbital Order-Disorder in Perovskite-like Coordination Polymers*

12^{30} : 14^{00} kosilo

14^{00} : 14^{20} K. Griffith: *High-rate Operando Synchrotron X-ray Diffraction, Solid-State NMR and X-Ray Spectroscopy, and Transition State Searching DFT of Non-nanostructured Oxides for Energy Storage*

14^{20} : 14^{40} H. Auer: *Characterizing Si/Ge/Sn-H Bonds In Zintl Phases by Diffraction, NMR and Calculations*

14^{40} : 15^{30} M. Perc (zunanje predavanje): *Tales About the Century of Physics and a Millennium of Art*

15^{30} : 16^{00} odmor za kavo

16^{00} : 16^{20} S. Radhakrishnan: *NMR Crystallography Guided Synthesis of Hyper-Crystalline ZnAl-CO_3 LDH*

16^{20} : 16^{40} C. Tschense: *A Software for Combining Structural Modeling, Computational Chemistry and Evaluation of NMR Experiments*

četrtek, 6. september 2018

$9^{00} : 9^{50}$	F.-X. Coudert (planarno predavanje): *Flexibility, Defects and Disorder in Soft Porous Crystals*
$9^{50} : 10^{10}$	A.-C. Pöppler: *Efavirenz Encapsulated Into Polypeptoid Micelles – "Insights" from Solid-State NMR, Quantum Chemical Calculations and Complementary Techniques*
$10^{10} : 10^{30}$	M. Evans: *SnP Anodes for Potassium-Ion Batteries: Insights from Computational Structure Prediction*
$10^{30} : 11^{00}$	odmor za kavo
$11^{00} : 11^{20}$	M. Baias: *NMR Crystallography Advancements for Exploring Polymorphism*
$11^{20} : 11^{40}$	Z. Berkson: *Framework Structures and Heteroatom Sites of the Zeolite Catalyst SSZ-70 Established by DNP-NMR and Synchrotron XRPD*
$11^{40} : 12^{00}$	T. Kemnitzer: *Exploring Adsorption Sites Inside CAU-1 Using Hyperpolarized ^{129}Xe NMR Spectroscopy*
$12^{00} : 12^{20}$	K. Asselman: *NMR Crystallography to Resolve Structure, Host-Guest and Guest-Guest Interactions in TMA Templated FAU Zeolite*