DGK conference 2022

Tuesday, 15 March 2022

Postersession: I (16:15 - 18:15)

[id] title	presenter	board
[11] Cation order determination in kesterite type quaternary semiconductors by Multiple Edge Anomalous Diffraction (MEAD)	TÖBBENS, Daniel	
[51] Elastic properties of dolomite-ankerite solid solutions	PENNACCHIONI, Lea	
[65] Negative thermal expansion, thermodynamic properties and temperature dependent Raman scattering of a new metal-organic perovskite framework [C(NH$_2$)$_3$][Ca(HCOO)$_3$]	HAUSSÜHL, Eiken	
[33] High-pressure crystal structures of Wadsley-type vanadium oxides V2O5 and V6O13	HAKALA, Viliam	
[13] Crystal structure for new coordination polymer obtained via solvothermal synthesis in Berghof autoclave	KOCHEL, Andrzej	
[29] Polymorphism in Cu20Te11Cl3	VOGEL, Anna	
[55] Cu3SeyTe1-y: A new representative of transition metal dichalcogenides	RABENBAUER, Alfred	
[79] The Powder Diffraction and Total Scattering Beamline P02.1 at PETRA III, DESY	SAN JOSE MENDEZ, Alba	
[141] Developments in High Pressure Clamp Cells for Neutron Scattering at the MLZ	GRZECHNIK, Andrzej	
[209] Squeezing the Most Data out of Your High-Pressure Experiment	GRAF, Jürgen	
[127] Isolated [SiO4]4– Tetrahedra in the Chloride-Poor Oxosilicate Ce3Cl[SiO4]2	Mr LOCKE, Ralf Jules Christian	
[157] Science communication as an important aspect of promoting research to the public	Dr KALIWODA, Melanie	
[83] Fine-tuning solid state luminescence properties of molecular crystals via solid solution formation	Mr SARŠŪNS, Kristaps	
[69] The benefits of Cu k-beta radiation for the single crystal X-ray structure determination of crystalline sponges	MEURER, Florian	
[225] Crystal structures of host-guest complexes of carboxylated pillar[5]arene with drugs	BUTKIEWICZ, Helena	
[221] Elucidation of Barocaloric Effect in Spin Crossover Compounds	SHAHED, Hend	
[231] Anion size dependence of band gaps of iodido antimonates	MÖBS, Jakob	
[223] Finite and Infinite Chains of Heavy-Atom Clusters	HERZ, Maria Annette	
[227] Influence of the Co to Mo molar ratio on active phase formation of ammonia synthesis catalysts: in-situ XRPD analysis	Mr ADAMSKI, Paweł	
[229] Topochemical conversion of layered tungstates: an in-situ Raman spectroscopy and total scattering study	LEFELD, Niels	
[91] Real-time investigation of Lysozyme crystallization kinetics: a neutron diffraction study	SCHRADER, Tobias	
[153] Perylene-based metal-organic frameworks for photochemical applications	Mr DEGER, Simon	

[195] Engineered crystals as a Racemate-to-Homochiral approach: chirality manipulation towards chiral resolution and the design of novel solid forms.	DE SOUSA CARVALHO JÚNIOR, Paulo	
[73] Halogenide-sodalites: Thermal expansion, decomposition and the Lindemann criterion	WOLPMANN, Marius	
[117] Review of symmetry and structure relationships of the stage-I graphite intercalation compounds (GICs) structure family	SEIDLMAYER, Stefan	
[185] Influence of Si on Hydrogen adsorption in SMoSe Janus host layer	VALLINAYAGAM, Muthu	
[71] Quantum crystallographic evaluation of the YLID crystal structure; reconsidering data quality	BALMOHAMMADI, Yaser	
[135] Structure prediction and behavior of (un)known materials in extreme conditions	ZAGORAC, Dejan	
[139] Structure prediction using global optimization and data mining in new Ce-O-N compounds	Dr ZAGORAC, Jelena	
[77] Evaluation of surrogate-models for the incorporation of tetravalent actinides in monazite phases	LENDER, Theresa	
[103] A49Tl108 (A = K, Rb), Beispiele für ternäre Trielide des K49Tl108-Strukturtyps	Mr LEHMANN, Bernard	
[119] High-Pressure Synthesis of Intermetallic Framework Compounds RESi3	NEZIRAJ, Teuta	
[123] A rare phenomenon inversion in mullite-type RAlGeO5 for R = Y, Sm – Lu	GHOSH, Kowsik	
[131] Synthesis and characterization of indium-containing sillenite	HOSSAIN, Md. Imran	
[133] Neue intermetallische Phasen der Systeme Ba--Mg--Zn und Ba--Mg--Cd	RÖHR, Caroline	
[149] Spectroscopic and structural characterization of molecular organic frameworks for heterogeneous catalysis	Mrs KAPPEL, Isabella	
[155] Rb4CuSb2Br12: A new vacancy-ordered quadruple perovskite	DAUB, Michael	
[175] Expansion of the hydride chemistry – new materials based on mixed anionic hydrides	MUTSCHKE, Alexander	
[193] From binary to ternary amalgams: expanding the structural variety of the Gd₁₄Ag₅₁ structure family	Mr HOHL, Timotheus	
[181] Pseudosymmetry in Cesium Orthotantalate(V)	ZAYTSEVA, Irina	
[199] Hundreds of starting points to develop protein-protein interaction modulators	BARTHEL, Tatjana	
[47] Ultrasmall covalently functionalized gold nanoparticles for protein targeting	KLEIN, Kai	
[125] Uncovering novel drug targets of polyprotein precursors of SARS-CoV2	FREIHERR VON SCHOLLEY, Gian Luca	

Wednesday, 16 March 2022

Postersession: II (16:45 - 18:45)

[id] title	presenter	board
[72] The In-Situ GIXS Heuristic Tool for Efficient Reduction of 2D Grazing-Incidence Data	REB, Lennart	
[180] The latest X-ray analysis solutions from Anton Paar	JONES, Andrew	
[116] Advances in the Parameter Space Concept for Crystal Structure Determination – a maximum resolution study	Dr ZSCHORNAK, Matthias	
[130] The Macromolecular Neutron Single Crystal Diffractometer BIODIFF for Proteins at the Heinz Maier-Leibnitz Zentrum	OSTERMANN, Andreas	
[38] Solid solution of lamellar metal-metal hydroxi salts with varying interlayer anions borate, chloride and sulfate containing different water contents	Prof. PÖLLMANN, Herbert	
[68] Synthesis and phase analysis of the polycrystalline K3Cu3AlO2(SO4)4	REITBERGER, Niclas	
[138] Element replacement in Mo2Ga2C via molten salt synthesis	SCHWEINLE, Catherine Fabienne	
[222] Synthesis of Polycrystalline Mixed System Rb3-xKxCu3AlO2(SO4)4	SCHEIBLICH, Clemens	
[58] In situ GIWAXS analysis of MAPbI3 formation using the software tool INSIGHT	REUS, Manuel	
[84] Lithium and electrolyte distribution in fresh and aged 18650-type lithium-ion batteries	PETZ, Dominik	
[160] Effects of soft mechanochemical synthesis in MAPbCl3 powders	SCHUCK, Götz	
[220] Probing Possible Non-Covalent Interactions on a Hexacationic Ag(I)-Pillarplex-Dodecyldiammonium Pseudo-Rotaxane as Terephthalate Salt	HEIDECKER, Alexandra	
[224] A Periodic Density Source for a Periodic System: Using PAW-DFT for Hirshfeld Atom Refinement	RUTH, Paul Niklas	
[226] Mechanically plastic molecular crystals for shapeable optic waveguide	Mr FEILER, Torvid	
[232] Hydrogen shift in electrostatic potential maps from 3D ED experiments	KLAR, Paul Benjamin	
[228] XRPD and TEM as tools to determine crystallite size of nanocrystalline iron	ALBRECHT, Aleksander	
[234] Crystal structure for new coordination polymer obtained via solvothermal synthesis in Berghof autoclave	KOCHEL, Andrzej	
[178] Anisotropic magnetoresistance and Magnetic properties of epilayers-perovskite LBMTO	OUMEZZINE, Marwène	
[86] Structural behavior of delithiated LixNi0,8Co0,15Al0,05O2 (0<x<1) battery cathodes	HÖLDERLE, Tobias	
[16] Stimulated Raman scattering in potassium nitrate, alpha-KNO3	BECKER-BOHATÝ, Petra	
[162] Magnetic phase diagram in rare-earth orthoferrite HoFeO3 from single crystal neutron diffraction in external magnetic field.	OVSIANIKOV, Aleksandr	
[172] Structure relations in the family of the solid solution Hf_xZr_{1-x}O_2	NENTWICH, Melanie	
[198] Towards a mechanistic understanding of the 2PI-2PI photo-addition of cinnamic acid compounds	STAMMLER, Felix Justus SCHRADER, Tobias	
[200] Electronic structure of the homologous series of Ruddlesden-Popper phases SrO(SrTiO3) , (= 0 - 3, ∞)	LUDT, Christian	

[152] Role of lithium diffusion on thermal expansion of Li0.4WO3 bronze studied by neutron elastic and quasi-elastic scatterings	MURSHED, M. Mangir	
[14] On the architecture of multicore iron oxide nanoparticles	NEUMANN, Stefan	
[216] Tuning the structural and magnetic properties of iron oxide nanoparticles	SUN, Xiao	
[24] Structural characterization of the solid solution Cu$_{2}$Mn(Ge$_{x}$Sn$_{1-x}$)S$_{4}$	MATZDORFF, David	
[66] Charge-Density Analysis of a disordered Aluminium Dihydrite Complex	KÖHLER, Christian	
[70] Characterization of the Delafossite solid solution series NaYb1–xLuxS2	HÄUSSLER, Ellen	
[88] Characterization of the formation of single-phase precious metal high entropy alloys by in situ diffraction	WEDEK, Lena Marie	
[96] Copper(I)-Based Pillarplexes: Platforms for Supramolecular Assemblies with Intrinsic Reactivity	PICKL, Thomas	
[104] Na7RbTl4: New Ternary Alkali Metal Thallide including Tl4(8-) tetrahedra	SCHWINGHAMMER, Vanessa	
[112] Electron density studies on a Cobalt Single-Molecule Magnet	Mrs RACHUY, Katharina	
[114] Zur Systematik der Strukturchemie von Dimetallaten A6[M 2Q6] mit Tetraederdimeren; Eine Vervollständigung der Dialuminate A6[Al2 Q6] (A=K, Rb, Cs; Q=S, Se, Te)	SCHWARZ, Michael	
[118] Sm7F12Cl2: Synthesis and Crystal Structure of a New Fluoride-Rich Samarium(II) Fluoride Chloride	Mr BUYER, Constantin	
[122] Synthesis and characterization of mullite-type NdMnTiO5: Structural, spectroscopic, thermal and magnetic properties analyses	GHOSH, Kowsik	
[124] Electrostatic self-assembly of p-sulfonatocalix[4]arene and pillar[n]pyridiniums into organic crystals	Mrs KRAVETS, Kateryna	
[126] Closing Some Gaps of Knowledge: Single Crystals of Pr2O[SiO4] und Sm2O[SiO4] with the A-Type Structure	DJENDJUR, Patrik	
[128] SmBi2O4Cl: The First Single-Crystal Study in the Systems LnBi2O4X	Mrs KURZ, Melanie	
[154] Effect of iron substitution by nickel on crystal structures, optical, and magnetic properties in double perovskite series Sr2Fe1-xNixTeO6 with x = 0, 0.25, 050, 0.75, and 1	ZARAQ, Asmaa	
[132] Structural and spectroscopic properties of SnMBO4 (M = Al, Ga)	WITTMANN, Sarah	
[144] Crystallized Pb(II)- and Sn(II)-ammine complexes as intermediates from the interaction of CH3NH2 with BX2 and CH3NH3BX3 (B = Pb, Sn; X = I, Br, Cl)	KRUMMER, Michael	
[156] New Hybrid Halogenobismuthates as Candidates for Non-linear Optical Properties	EBLE, Kevin	
[164] Controlling the bonding situation of tetryliumylidenes with Ni(0) centers by denticity of the ligand scaffold	KEIL, Philip	
[168] The crystal structure of single crystalline PrCa4O[BO3]3	WEIGEL, Tina	
[204] A newly crystallized structure of human formylglycine-generating enzyme	KOWAL, Julia L.	