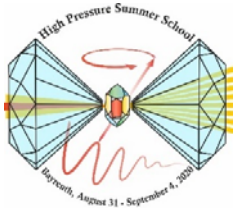

Deutsche Gesellschaft für Kristallographie

IUCr

IUCr/DGK Summer School 2020, Bayreuth, Germany

"Introduction to Novel Methods of Atomic and Electronic Structure Studies at High Pressures"

Time (CEST)*	Monday, Aug. 31st	Tuesday, Sept. 1st	Wednesday, Sept. 2nd	Thursday, Sept. 3rd	Friday, Sept. 4th
8.15-8.30	**Opening Remarks**				
8.30-9.30	Basics of DACs Pressure determination Equation of state (**LSD**)	Acquiring good X-ray diffraction SC data in DACs (**DL**)	Hands-on: Simple cases with CrysalisPro (**DL, SK, AS, LSD**) *4 groups in parallel*	Hands-on: Structure solution and refinement (**DL, SK, AS, LSD**) *4 groups in parallel*	Hands-on: Mapping and analysis of complex samples (**DL, SK, AS, LSD**) *4 groups in parallel*
9.30-10.30	Introduction to crystal symmetry (**LSD**)	PETRA III facility, the P02.2 beamline and the SC crystal data setup (**KG**)	Hands-on: More complex cases with CrysalisPro (**DL, SK, AS, LSD**) *4 groups in parallel*	Hands-on: Structures solution/refinements (**DL, SK, AS, LSD**) *4 groups in parallel*	Processing HP data: problems and helpful tools for their solution (**KF**)
10.30-11.30	Introduction to X-ray diffraction (**DL**)	Introduction to the CrysalisPro software (**LSD**)	Introduction to Jana2006 (installation etc.) (**KG**)	Application Case – material sciences (**SO**)	Combination of NMR and SC data for Materials Science (**TM**)
11.30-12.30	Introduction to NMR (**TM**)	Technical aspects of HP NMR (**TM**)	HP NMR methods (**TM**)	Hands-on: NMR **group II** (**TM**)	Hands-on: NMR **group III** (**TM**)
12:30-13:30	LUNCH	LUNCH	LUNCH	LUNCH	LUNCH
13.30-14.30	Heating (**LSD**) and cooling (**KG**) in DACs	Hands-on: CrysalisPro (installation, calibration, …) (**DL, SK, AS, LSD**) *4 groups in parallel*	Hands-on: NMR **group I** (**TM**)	Handling twinned crystals data (**EB**)	SC data validation (**EB**)
14.30-15.30	Historical overview and perspectives of HP crystallography **(ND)**	Crystal structure visualization and building blocks of HP crystallochemistry **(LSD)**	APS facility, the GSECARS beamline (**VP** or/and **SC**)	Getting the maximum out of your SC data (**MB**)	Application Case – High-pressure nitrides (**MB**)
15.30-15.45					**Concluding Remarks**

There will be 5 min breaks at 9.25, 13.25 and 10 min breaks at 10.20 and 14.20

ND - Natalia Dubrovinskaia, DL - Dominique Laniel, TM - Thomas Meier, KG - Konstantin Glazyrin, SK - Saiana Khandarkhaeva, AS - Achim Schaller, VP - Vitali Prakapenka, SC - Stella Chariton, SO - Sergey Ovsyannikov, EB - Elena Bykova, MB - Maxim Bykov, KF - Karen Friese, LSD - Leonid Dubrovinsky