

6th EUROPEAN CRYSTALLOGRAPHIC SCHOOL

ECS6

4 - 10 July 2021 / online from Budapest, Hungary

Final Programme

(All times are in the GMT +2 time zone)

Sunday / 4 July 2021

14:30	16:00	Speakers' information
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Monday / 5 July 2021

Monday session 1

8:40	8:45	Opening of ECS6, welcome and technical information	Petra Bombicz <i>Chair of ECS6</i>	Chemical Crystallography Research Laboratory Research Centre for Natural Sciences Budapest, Hungary
8:45	8:50	Opening remarks	Udo Heinemann <i>President of the ECA</i>	Max-Delbrück-Centrum für Molekulare Medizin und Institut für Chemie und Biochemie Freie Universität Berlin Berlin, Germany
8:50	9:00	The role of the IUCr in crystallography	Brian McMahon	International Union of Crystallography Chester, United Kingdom
9:00	9:30	The Cambridge Structural Database - Learning from one million crystal structures	Suzanna Ward and Ilaria Gimondi	Cambridge Crystallographic Data Centre Cambridge, United Kingdom
9:30	9:55	The Protein Data Bank - 50 years and counting	David Armstrong	Protein Data Bank in Europe Hinxton, United Kingdom
9:55	10:10	Questions & answers with Brian McMahon, Suzanne Ward and Ilaria Gimondi, David Armstrong / Moderator: Nikolettá Báthori		

10:10	10:30	Coffee break
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Monday session 2

10:30	11:45	Diffraction physics	Gyula Faigel	Wigner RCP of the Hungarian Academy of Sciences Budapest, Hungary
11:45	12:00	Questions & answers with Gyula Faigel / Moderator: Gábor Bortel		

12:00	13:00	Lunch break
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Monday session 3

13:00	14:15	Crystals and symmetry – How to use the International Tables for Crystallography (Volume A)	Christian Lehmann	Max-Planck-Institut für Kristallographie Mülheim an der Ruhr, Germany
14:15	14:30	Questions & answers with Christian Lehmann / Moderator: Gábor Bortel		
14:30	15:30	Theory and Laboratory practice (SAXS): András Wacha: Small-Angle X-ray Scattering: A Complementary technique to diffraction		
15:30	16:00	Question & answers: Theory and Laboratory practice (SAXS) with András Wacha / Moderator: John R. Helliwell		
16:00	16:20	Coffee break		
Monday session 4				
16:20	17:00	Reciprocal space	Gábor Bortel	Wigner Research Centre for Physics Budapest, Hungary
17:00	17:10	Questions & answers with Gábor Bortel / Moderator: Gyula Faigel		
17:10	17:55	Data collection strategy	Tobias Stürzer	Bruker AXS GmbH Karlsruhe, Germany
17:55	18:10	Questions & answers with Tobias Stürzer / Moderator: Horst Puschmann		
18:10	19:00	Networking / Welcome drink & chat		

Tuesday / 6 July 2021

Tuesday session 1				
8:40	9:05	Instrumentation, sources and detectors	John R. Helliwell	School of Chemistry University of Manchester Manchester, United Kingdom
9:05	9:55	Why should you know about X-ray detectors?	Dubravka Sisak Jung	Dectris Ltd. Baden, Switzerland
9:55	10:10	Questions & answers with John R. Helliwell, Dubravka Sisak Jung / Moderator: András Wacha		
10:10	10:30	Coffee break		
Tuesday session 2				
10:30	11:10	Overview lecture of the probes of the structure of matter; X-rays, neutrons and electrons	John R. Helliwell	University of Manchester Faculty of Science and Engineering Manchester, United Kingdom
11:10	11:45	X-ray Free Electron Lasers: A new paradigm in science	Robert Feidenhans'l	European XFEL GmbH Schenefeld, Germany
11:45	12:00	Questions & answers with John R. Helliwell, Robert Feidenhans'l / Moderator: Gyula Faigel		
12:00	13:00	Lunch break		
Tuesday session 3				
13:00	13:25	Crystallisation - A very practical guide to getting that perfect single crystal	Nikoletta Báthori	Chemistry Department Cape Peninsula University of Technology Cape Town, South Africa

13:25	13:50	Protein crystallization	Veronika Harmat	Laboratory of Structural Chemistry and Biology Institute of Chemistry Eötvös Loránd University Budapest, Hungary
13:50	14:15	“With a little help from my friends”: complementary techniques to get to know your crystal structure better	Chiara Massera	Department of Chemistry University of Parma Parma, Italy
14:15	14:30	Questions & answers with Nikolettá Bátori, Veronika Harmat, Chiara Massera / Moderator: Laura Bereczki		
14:30	15:30	Laboratory practice (SXR) / Tamás Holczbauer, Gábor Bortel, Nóra May, Laura Bereczki, Éva Kováts, Sourav De, Petra Bombicz: Small molecule X-ray diffraction		
15:30	16:00	Question & answers: Laboratory practice (SXR) / Moderator: Tamás Holczbauer		
16:00	16:20	Coffee break		
Tuesday session 4				
16:20	17:00	From raw diffraction data to refined single crystal structures	Christian Lehmann	Max-Planck-Institut für Kristallographie Mülheim an der Ruhr, Germany
17:00	17:10	Questions & answers with Christian Lehmann / Moderator: Dubravka Sisak-Jung		
17:10	18:10	Poster session and flash presentations I.		
18:15	19:15	Networking / Virtual sightseeing of the Buda Castle		

Wednesday / 7 July 2021

Wednesday session 1				
8:40	9:55	Macromolecular structure determination by X-ray crystallography (Part I)	Manfred Weiss	Helmholtz-Zentrum Berlin Berlin, Germany
9:55	10:10	Questions & answers with Manfred Weiss / Moderator: Veronika Harmat		
10:10	10:30	Coffee break		
Wednesday session 2				
10:30	11:45	Macromolecular structure determination by X-ray crystallography (Part II)	Manfred Weiss	Helmholtz-Zentrum Berlin Berlin, Germany
11:45	12:00	Questions & answers with Manfred Weiss / Moderator: Vilmos Fülöp		
12:00	13:00	Lunch break		
Wednesday session 3				
13:00	13:38	Enzymes involved in key biomedical processes	Beáta Vértessy	Department of Applied Biotechnology and Food Science Budapest University of Technology and Economics and Laboratory of Genome Metabolism and Repair Institute of Enzimology Budapest, Hungary

13:38	14:15	Model building and electron density maps - howtos in protein crystallography	Veronika Harmat	Laboratory of Structural Chemistry and Biology Institute of Chemistry Eötvös Loránd University Budapest, Hungary
14:15	14:30	Questions & answers with Beáta Vértessy, Veronika Harmat / Moderator: Manfred Weiss		
14:30	15:30	Laboratory practice (Macromol 1) / Ibolya Leveles, Veronika Harmat: Protein crystallization and data collection		
15:30	16:00	Question & answers: Laboratory practice (Macromol 1) / Moderator: Veronika Harmat		
16:00	16:20	Coffee break		
Wednesday session 4				
16:20	16:35	Validating the results of small molecule single crystal structure analysis	Christian Lehmann	Max-Planck-Institut für Kristallographie Mülheim an der Ruhr, Germany
16:35	16:50	Validating the results of macromolecule single crystal structure analysis	Manfred Weiss	Helmholtz-Zentrum Berlin Berlin, Germany
16:50	17:05	Data validation	John R. Helliwell	University of Manchester Faculty of Science and Engineering Manchester, United Kingdom
17:05	17:10	Questions & answers with Christian Lehmann, Manfred Weiss, John R. Helliwell / Moderator: Attila Bényei		
17:10	17:35	Data preservation and quality: FAIR and FACT in crystallography	John R. Helliwell	University of Manchester Faculty of Science and Engineering Manchester, United Kingdom
17:35	18:00	Equilibrium studies to reveal stability, composition and structure in solution	Éva A. Enyedy	Department of Inorganic and Analytical Chemistry University of Szeged Szeged, Hungary
18:00	18:10	Question & answers with John R. Helliwell, Éva A. Enyedy / Moderator: Nóra May		
18:10	19:15	Networking / Concert of Chemical Singers		

Thursday / 8 July 2021

Thursday session 1				
8:40	9:05	Disorder and twinning	László Fábán	School of Pharmacy University of East Anglia Norwich, United Kingdom
9:05	9:30	X-ray diffraction as absolute method to determine absolute configuration	Attila Bényei	University of Debrecen Institute of Chemistry Debrecen, Hungary
9:30	9:55	Structure determination from powder diffraction data	László Fábán	School of Pharmacy University of East Anglia Norwich, United Kingdom
9:55	10:10	Question & answers with László Fábán, Attila Bényei / Moderator: Andrzej Katrusiak		
10:10	10:30	Coffee break		

Thursday session 2				
10:30	11:08	Polymorphism of solid state structures and its consequences	Attila Béneyei	University of Debrecen Institute of Chemistry Debrecen, Hungary
11:08	11:45	Polymorphism and isostructurality	Petra Bombicz	Chemical Crystallography Research Laboratory Research Centre for Natural Sciences Budapest, Hungary
11:45	12:00	Questions & answers with Attila Béneyei, Petra Bombicz / Moderator: Nikolettá Báthori		
12:00	13:00	Lunch break		
Thursday session 3				
13:00	14:15	Is structural characterization important in the study of Metal Organic Frameworks, bio-MOFs and polymorphs? No doubt about that!	Teresa Duarte	Instituto Superior Técnico Universidade de Lisboa Lisbon, Portugal
14:15	14:30	Questions & answers with Teresa Duarte / Moderator: Ilaria Gimondi		
14:30	15:30	Laboratory practice (Olex2): Horst Puschmann: Solving and refining small-molecule structures using Olex2		
15:30	16:00	Question & answers: Laboratory practice (Olex2) with Horst Puschmann / Moderator: Chiara Massera		
16:00	16:20	Coffee break		
Thursday session 4				
16:20	17:00	Powder Diffraction with single-crystal instruments	Christian J. Schürmann	Rigaku Europe SE Göttingen, Germany
17:00	17:10	Questions & answers with Christian J. Schürmann / Moderator: Attila Béneyei		
17:10	18:10	Poster session and flash presentations II.		
18:10	19:00	Networking / Quiz & chat		

Friday / 9 July 2021

Friday session 1				
8:40	9:55	Stuctural aspects of COVID-19	Vilmos Fülöp	University of Warwick Coventry, United Kingdom
9:55	10:10	Question & answers with Vilmos Fülöp / Moderator: Manfred Weiss		
10:10	10:30	Coffee break		
Friday session 2				
10:30	11:45	Crystallography in extreme conditions	Andrzej Katrusiak	Faculty of Chemistry Adam Mickiewicz University Poznan, Poland
11:45	12:00	Questions & answers with Andrzej Katrusiak / Moderator: Éva Kováts		

12:00	13:00	Lunch break		
Friday session 3				
13:00	14:15	Noncovalent interactions at work	Giancarlo Terraneo	Politecnico di Milano Milan, Italy
14:15	14:30	Questions & answers with Giancarlo Terraneo / Moderator: Petra Bombicz		
14:30	15:30	Laboratory practice (Macromol 2): Veronika Harmat, Ibolya Leveles: Solving protein structures with X-ray crystallography		
15:30	16:00	Question & answers: Laboratory practice (Macromol 2) / Moderator: Ibolya Leveles		
16:00	16:20	Coffee break		
Friday session 4				
16:20	17:00	Electron crystallography	Enrico Mugnaioli	Center for Nanotechnology Innovation@NEST Istituto Italiano di Tecnologia Pisa, Italy
17:00	17:10	Questions & answers with Enrico Mugnaioli / Moderator: John R. Helliwell		
17:10	17:50	How to publish your research	Mike Andrews	Royal Society of Chemistry London, United Kingdom
17:50	18:00	Question & answers with Mike Andrews / Moderator: Suzanna Ward		
18:10	19:00	Closing ceremony / Poster prizes / Goodbye drink & chat		

Saturday / 10 July 2021

20:45	21:40	Virtual sunset bike tour in Budapest		
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