

# 6th EUROPEAN CRYSTALLOGRAPHIC SCHOOL

## ECS6

4 - 10 July 2021 / online from Budapest, Hungary

### Final Programme\*

#### Sunday / 4 July 2021

14:30 16:00 **Speakers' information**

#### Monday / 5 July 2021

Time zone: GMT +2

##### Monday session 1

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

10:10 10:30 **Coffee break**

##### Monday session 2

10:30	11:45	<b>Diffraction physics</b>	<b>Gyula Faigel</b>	Hungarian Academy of Sciences Budapest, Hungary
11:45	12:00	<b>Questions &amp; answers (Gyula Faigel)</b>		

12:00 13:00 **Lunch break**

##### Monday session 3

13:00	14:15	<b>Crystals and symmetry – How to use the International Tables for Crystallography (Volume A)</b>	<b>Christian Lehmann</b>	Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr, Germany
14:15	14:30	<b>Questions &amp; answers (Christian Lehmann)</b>		
14:30	15:30	<b>Theory and Laboratory practice (SAXS): András Wacha: Small-Angle X-ray Scattering: A complementary technique to diffraction</b>		
15:30	16:00	<b>Question &amp; answers (Theory and Laboratory practice (SAXS))</b>		
16:00	16:20	<b>Coffee break</b>		

**Monday session 4**

16:20	17:00	<b>Reciprocal space</b>	<b>Gábor Bortel</b>	Wigner Research Centre for Physics Budapest, Hungary
17:00	17:10	<b>Questions &amp; answers (Gábor Bortel)</b>		
17:10	17:55	<b>Data collection strategy</b>	<b>Tobias Stürzer</b>	Bruker AXS GmbH Karlsruhe, Germany
17:55	18:10	<b>Questions &amp; answers (Tobias Stürzer)</b>		
18:10	19:00	<b>Networking / Welcome drink &amp; chat</b>		

**Tuesday / 6 July 2021****Tuesday session 1**

8:40	9:05	<b>Instrumentation, sources and detectors</b>	<b>John R. Helliwell</b>	School of Chemistry University of Manchester Manchester, United Kingdom
9:05	9:55	<b>Why should you know about X-ray detectors?</b>	<b>Dubravka Sisak Jung</b>	XRD Application Scientist DECTRIS Ltd. Baden, Switzerland
9:55	10:10	<b>Questions &amp; answers (John R. Helliwell, Dubravka Sisak Jung)</b>		
10:10	10:30	<b>Coffee break</b>		

**Tuesday session 2**

10:30	11:10	<b>Overview lecture of the probes of the structure of matter; X-rays, neutrons and electrons</b>	<b>John R. Helliwell</b>	School of Chemistry University of Manchester Manchester, United Kingdom
11:10	11:45	<b>X-ray Free Electron Lasers: A new paradigm in science</b>	<b>Robert Feidenhans'l</b>	European XFEL GmbH Schenefeld, Germany
11:45	12:00	<b>Questions &amp; answers (John R. Helliwell, Robert Feidenhans'l)</b>		
12:00	13:00	<b>Lunch break</b>		

**Tuesday session 3**

13:00	13:25	<b>Crystallisation - A very practical guide to getting that perfect single crystal</b>	<b>Nikoletta Bátori</b>	Chemistry Department Cape Peninsula University of Technology Cape Town, South Africa
13:25	13:50	<b>Protein crystallization</b>	<b>Veronika Harmat</b>	Laboratory of Structural Chemistry and Biology Institute of Chemistry Eötvös Loránd University Budapest, Hungary
13:50	14:15	<b>"With a little help from my friends": complementary techniques to get to know your crystal structure better</b>	<b>Chiara Massera</b>	Department of Chemistry University of Parma Parma, Italy
14:15	14:30	<b>Questions &amp; answers (Nikoletta Bátori, Veronika Harmat, Chiara Massera)</b>		
14:30	15:30	<b>Laboratory practice (SXR) / Tamás Holczbauer, Gábor Bortel, Nóra May, Laura Bereczki, Éva Kováts, Sourav De, Petra Bombicz: Small molecule X-ray diffraction</b>		
15:30	16:00	<b>Question &amp; answers (Laboratory practice (SXR))</b>		
16:00	16:20	<b>Coffee break</b>		

**Tuesday session 4**

16:20	17:00	<b>From raw diffraction data to refined single crystal structures</b>	<b>Christian Lehmann</b>	Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr, Germany
17:00	17:10	<b>Questions &amp; answers (Christian Lehmann)</b>		
17:10	18:10	<b>Poster session and flash presentations I.</b>		
18:15	19:15	<b>Networking / Virtual sightseeing of the Buda Castle</b>		

## Wednesday / 7 July 2021

### Wednesday session 1

8:40	9:55	<b>Macromolecular structure determination by X-ray crystallography (Part I)</b>	<b>Manfred Weiss</b>	Helmholtz-Zentrum Berlin Berlin, Germany
9:55	10:10	<b>Questions &amp; answers (Manfred Weiss)</b>		
10:10	10:30	<b>Coffee break</b>		

### Wednesday session 2

10:30	11:45	<b>Macromolecular structure determination by X-ray crystallography (Part II)</b>	<b>Manfred Weiss</b>	Helmholtz-Zentrum Berlin Berlin, Germany
11:45	12:00	<b>Questions &amp; answers (Manfred Weiss)</b>		
12:00	13:00	<b>Lunch break</b>		

### Wednesday session 3

13:00	13:38	<b>Enzymes involved in key biomedical processes</b>	<b>Beáta Vértessy</b>	Department of Applied Biotechnology and Food Science Budapest University of Technology and Economics and Laboratory of Genome Metabolism and Repair Institute of Enzymology Budapest, Hungary
13:38	14:15	<b>Model building and electron density maps - howtos in protein crystallography</b>	<b>Veronika Harmat</b>	Laboratory of Structural Chemistry and Biology Institute of Chemistry Eötvös Loránd University Budapest, Hungary
14:15	14:30	<b>Questions &amp; answers (Beáta Vértessy, Veronika Harmat)</b>		
14:30	15:30	<b>Laboratory practice (Macromol 1) / Ibolya Leveles, Veronika Harmat: Protein crystallization and data collection</b>		
15:30	16:00	<b>Question &amp; answers (Laboratory practice (Macromol 1))</b>		

### Wednesday session 4

16:20	16:35	<b>Validating the results of small molecule single crystal structure analysis</b>	<b>Christian Lehmann</b>	Max-Planck-Institut für Kohlenforschung Mülheim an der Ruhr, Germany
16:35	16:50	<b>Validating the results of macromolecule single crystal structure analysis</b>	<b>Manfred Weiss</b>	Helmholtz-Zentrum Berlin Berlin, Germany
16:50	17:05	<b>Data validation</b>	<b>John R. Helliwell</b>	School of Chemistry University of Manchester Manchester, United Kingdom
17:05	17:10	<b>Questions &amp; answers (Christian Lehmann, Manfred Weiss, John R. Helliwell)</b>		
17:10	17:35	<b>Data preservation and quality: FAIR and FACT in crystallography</b>	<b>John R. Helliwell</b>	School of Chemistry University of Manchester 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 (John R. Helliwell, Éva A. Enyedy)		
18:10	19:15	Networking / Concert of Chemical Singers		

## Thursday / 8 July 2021

<b>Thursday session 1</b>				
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 Béneyi	Department of Physical Chemistry University of Debrecen 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 (László Fábán, Attila Béneyi)		
10:10	10:30	Coffee break		
<b>Thursday session 2</b>				
10:30	11:08	Polymorphism of solid state structures and its consequences	Attila Béneyi	Department of Physical Chemistry University of Debrecen 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 (Attila Béneyi, Petra Bombicz)		
12:00	13:00	Lunch break		
<b>Thursday session 3</b>				
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	Centro de Química Estrutural Instituto Superior Técnico Lisbon, Portugal
14:15	14:30	Questions & answers (Teresa Duarte)		
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))		
16:00	16:20	Coffee Break		
<b>Thursday Session 4</b>				
16:20	17:00	Powder Diffraction with single-crystal instruments	Christian J. Schürmann	Rigaku Europe SE Göttingen, Germany
17:00	17:10	Questions & answers (Christian J. Schürmann)		
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	<b>Structural aspects of COVID-19</b>	<b>Vilmos Fülöp</b>	The University of Warwick Coventry, United Kingdom
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9:55	10:10	<b>Question &amp; answers (Vilmos Fülöp)</b>		
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10:10	10:30	<b>Coffee Break</b>		
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### Friday Session 2

10:30	11:45	<b>Crystallography in extreme conditions</b>	<b>Andrzej Katrusiak</b>	Faculty of Chemistry Adam Mickiewicz University Poznan, Poland
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11:45	12:00	<b>Questions &amp; answers (Andrzej Katrusiak)</b>		
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12:00	13:00	<b>Lunch Break</b>		
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### Friday Session 3

13:00	14:15	<b>Noncovalent interactions at work</b>	<b>Giancarlo Terraneo</b>	Laboratory of Supramolecular and BioNano Materials Chemistry, Materials, and Chemical Engineering Politecnico di Milano Milan, Italy
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14:15	14:30	<b>Questions &amp; answers (Giancarlo Terraneo)</b>		
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14:30	15:30	<b>Laboratory practice (Macromol 2): Veronika Harmat, Ibolya Leveles: Solving protein structures with X-ray crystallography</b>		
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15:30	16:00	<b>Question &amp; answers (Laboratory practice (Macromol 2))</b>		
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16:00	16:20	<b>Coffee Break</b>		
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### Friday Session 4

16:20	17:00	<b>Electron crystallography</b>	<b>Enrico Mugnaioli</b>	Center for Nanotechnology Innovation@NEST Istituto Italiano di Tecnologia Pisa, Italy
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17:00	17:10	<b>Questions &amp; answers (Enrico Mugnaioli)</b>		
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17:10	17:50	<b>How to publish your research</b>	<b>Mike Andrews</b>	CrystEngComm United Kingdom
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17:50	18:00	<b>Question &amp; answers (Mike Andrews)</b>		
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18:00	18:10	<b>Break</b>		
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18:10	19:00	<b>Closing ceremony / Poster prizes / Goodbye drink &amp; chat</b>		
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## Saturday / 10 July 2021

20:45	21:40	<b>Virtual sunset bike tour in Budapest</b>		
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\*The Organizers reserve the right to make changes in the programme!