MACSMIN 2026

Tuesday 26th May MIF boardroom	Wednesday 27th May MIF boardroom	Thursday 28th May CMD Seminar room	Friday 29th May MIF boardroom
10.00-10.45 Arrivals and registration	**9.00-9.45** John R. Helliwell *(University of Manchester, UK)* Precision and Accuracy in Biological Crystallography, Diffraction, Scattering, Microscopies, and Spectroscopies.	**09.00-09.45** Saulius Grazulis *(Crystallography Open Database, Vilnus, Lithuania)* Towards the catalogue of entangled nets and molecules in the COD and other open databases.	**09.00-09.45** Alex Wlodawer *(National Cancer Institute, US)* Community efforts to improve the contents of the Protein Data Bank, a crucial resource for structural biology.
10.45-11.00 Vitaliy Kurlin *(Liverpool, UK)* Opening: history and vision of MACSMIN	**10.00-10.45** Thérèse Malliavin *(University of Lorraine, France)* Influence of Stereochemistry in a Local Approach for Calculating Protein Conformations.	**10.00-10.45** Wolfgang Hornfeck *(Institute of Physics, Czech Academy of Sciences)* Arithmetic and algebraic patterns in crystal structures.	**10.00-10.45** Ziqiu Jiang *(Liverpool, UK)* Atomic clashes in the Protein Data Bank (PDB).
11.00-11.45 Pavel Buividovich *(Liverpool, UK)* Hybrid Quantum Monte-Carlo algorithm for strongly correlated electrons and polaron-type problems.	**11.00-11.45** Alexandre de Brevern *(Université Paris Cité, France)* Protein Blocks as a discrete geometric model for protein conformational spaces.	**11.00-11.45** Yury Elkin *(Liverpool, UK)* A geometric map of chemical elements based on molecular databases QM9 and GEOM	**11.00-11.20** Jack Gallimore *(University of Leeds, UK)* Geometry based method for identifying hydrogen bonds and classifying helices. **11.30-11.50** Gabriel Newton *(Liverpool, UK)* ProtNRD: A 3D Ramachandran Dashboard for Exploring Neighbouring Residue Influences on Backbone Geometry.
Lunch VGM cafe (Victoria Gallery & Museum)	Lunch TBD	Lunch VGM cafe (Victoria Gallery & Museum)	Lunch VGM cafe (Victoria Gallery & Museum)

13.30-14.15 Alessandro Troisi *(Liverpool, UK)* High-Throughput exploration of molecular and polymer systems: status and emerging problems for data science.	**14.00-14.45** Olga Anosova *(Liverpool, UK)* Data Science exposed thousands of exact duplicates in high-profile structural databases.	**13.30-14.15** Daniel Widdowson *(Liverpool, UK)* The Crystal Geomap visualises materials databases in real time. **14.30-14.50** Surya Majumder (*Liverpool, UK)* Continuous invariant-based asymmetries of periodic crystals quantify deviations from higher symmetry.	
14.30-15.15 Greg McColm *(University of South Florida, US)* Combinatorial and Topological Equivalence of Representations of Crystals.	**15.00-15.45** Alexei Lisitsa *(Liverpool, UK)* Automated reasoning for knots and knotted structures with possible applications to proteins.	**15.00-15.45** Richard Catlow FRS *(UCL, UK)* Crystal and Nano-Structure Prediction: Achievements and Opportunities.	
15.30-16.15 Katerina Vriza *(GSK, UK)* Closing the loop between digital models and autonomous experimentation in chemical discovery.	**16.00-16.45** Pawel Rubach *(Warsaw School of Economics, Poland)* Knot or not? Identifying unknotted proteins in knotted families with sequence-based Machine Learning model.	**16.00-16.45** Simon Billinge *(University of California Santa Barbara, US)* Symmetry in a Hierarchical World	
17.00-18.00 Vitaliy Kurlin Geometric Data Science (inaugural lecture organised by the CSI school). **Elizabeth Gidney Room, top floor in the Liverpool Guild of Students**. **Please register here:**			
18.00-19.00 Reception (organised by the CSI school)	**18.00-21.00** Dinner Seven seas brasseries, the Liner hotel	**18.00-21.00** Dinner Seven seas brasseries, the Liner hotel	