

# MACSMIN 2026

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

<p><b>13.30-14.15</b>  <a href="#">Alessandro Troisi</a>  <i>(UoL, UK)</i>  High-Throughput exploration of molecular and polymer systems: status and emerging problems for data science.</p>	<p><b>14.00-14.45</b>  <a href="#">Olga Anosova</a>  <i>(UoL, UK)</i>  A classification of protein backbones by complete and bi-continuous invariants in linear time.</p>	<p><b>13.30-14.15</b>  <a href="#">Daniel Widdowson</a>  <i>(UoL, UK)</i>  The Crystal Geomap visualises materials databases in real time.</p> <p><b>14.30-14.50</b>  Surya Majumder  <i>(UoL, UK)</i>  Continuous invariant-based asymmetries of periodic crystals quantify deviations from higher symmetry.</p>	
<p><b>14.30-15.15</b>  <a href="#">Greg McColm</a>  <i>(University of South Florida, US)</i>  Combinatorial and Topological Equivalence of Representations of Crystals.</p>	<p><b>15.00-15.45</b>  <a href="#">Alexei Lisitsa</a>  <i>(UoL, UK)</i>  Automated reasoning for knots and knotted structures with possible applications to proteins.</p>	<p><b>15.00-15.45</b>  <a href="#">Richard Catlow</a> FRS  <i>(UCL, UK)</i>  Crystal and Nano-Structure Prediction: Achievements and Opportunities.</p>	
<p><b>15.30-16.15</b>  <a href="#">Katerina Vriza</a>  <i>(GSK, UK)</i>  Closing the loop between digital models and autonomous experimentation in chemical discovery.</p>	<p><b>16.00-16.45</b>  <a href="#">Pawel Rubach</a>  <i>(Warsaw School of Economics, Poland)</i>  Knot or not? Identifying unknotted proteins in knotted families with sequence-based Machine Learning model.</p>	<p><b>16.00-16.45</b>  <a href="#">Simon Billinge</a>  <i>(University of California Santa Barbara, US)</i>  TBA</p>	
<p><b>17.00-18.00</b>  <a href="#">Vitaliy Kurlin</a>  Geometric Data Science (inaugural lecture organised by the <a href="#">CSI school</a>).  <b>(Location: Elizabeth Gidney Room, top floor in the <a href="#">Liverpool Guild of Students</a>) Please <a href="#">register here</a>:</b></p> 			