Miloslav Torda, Ph.D.

CURRICULUM VITAE

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Professional Appointments

- **2023–Present**: Postdoctoral Research Associate, University of Liverpool
  - Principal Investigator: Prof. A. I. Cooper
- **2018–2023**: Postgraduate Researcher, University of Liverpool
  - Advisors: Prof. J. Y. Goulermas, Prof. V. Kurlin, and Prof. G. M. Day
- **2006–2010**: Automated Trading System Developer, MG-service, spol. s r.o., Košice

Education

- **2023**: Ph.D. in Computer Science, University of Liverpool, United Kingdom
  - Thesis title: *Maximally Dense Crystallographic Symmetry Group Packings for Molecular Crystal Structure Prediction Acceleration.*
  - Advisors: Prof. J. Y. Goulermas, Prof. V. Kurlin, and Prof. G. M. Day
- **2018**: M.Sc. in Probability Theory and Mathematical Statistics (Summa Cum Laude), Comenius University, Slovakia
- **2015**: B.Sc. in Mathematics, Comenius University, Slovakia
- **2006**: M.A. in Psychology, Faculty of Philosophy, Comenius University, Slovakia

Research Visits

- **May–June 2023**: Mathematical Institute, University of Jena, Germany

Publications

Journal Articles

- **2023**: **Torda, M.**, Goulermas, J. Y., Púček, R., and Kurlin, V. *Entropic Trust Region for Densest Crystallographic Symmetry Group Packings*. SIAM Journal on Scientific Computing, 45(4), B493–B522.
- **2022**: **Torda, M.**, Goulermas, J. Y., Kurlin, V., and Day, G. M. *Densest Plane Group Packings of Regular Polygons*. Physical Review E, 106(5), 054603.

Conference Proceedings

- **2018**: **Torda, M.** and Farkas, I. *Evaluation of Information-Theoretic Measures in Echo State Networks on the Edge of Stability*. In 2018 International Joint Conference on Neural Networks (IJCNN) (pp. 1–6). IEEE.

Talks

Invited Talks

- **2025**: *From Molecular Shape to Crystal Symmetry: Densest Packings of Radially Equilateral Molecules.* MACSMIN 2025: Mathematics and Computer Science for Materials Innovation, Materials Innovation Factory, University of Liverpool, UK, September 8-12.
- **2024**: *Geometric Perspectives on the Crystallization of Molecular Crystals: Crystallographic Symmetry Group Packings, Uniform Tessellations, and Molecular Frameworks.* Selected Topics in Mathematics Seminar (Online), November 29
- **2024**: *Geometry-Informed Programming: From Statistical Manifolds to Hard Packings of van der Waals Models.* Crystal Engineering (Gordon Research Seminar), Maine, USA, June 22–23
- **2024**: *Panel Discussion: Barriers to adoption of AI in the materials value chain* (Panelist). Materials Research Exchange 2024 – Materials & AI Sessions, Business Design Centre, London, UK, April 23

- **2023**: *Maximally Dense Crystallographic Symmetry Group Packings through Entropic Trust Region: An Information Geometric Perspective.* CaLISTA Kick-off Meeting, Department of Mathematics, University of Bologna, Italy, June 5–9
- **2023**: *Symmetries of Maximally Dense Plane Group Packings of Regular Convex Polygons.* Oberseminar Algebra, University of Jena, Germany, May 23
- **2019**: *Dense Periodic Packings in the Light of Crystal Structure Prediction* Soft Packings. Nested Clusters and Condensed Matter, Banff International Research Station, Casa Matemática Oaxaca, Mexico, September 29–October 4

Contributed Conference Talks

- **2021**: *Geometry of the n-Torus Stochastic Trust Region Method for Materials Discovery.* British Mathematical Colloquium (BMC) and British Applied Mathematics Colloquium (BAMC), Glasgow, UK, April 6–9
- **2019**: *Dense Periodic Packings in the Light of Crystal Structure Prediction.* AI3SD Network+ Conference, Holiday Inn Winchester & Winchester Science Centre, UK, November 18–19

Invited On-Campus Seminar Talks

- **2024**: *Geometric Modeling in the Prediction of Molecular Crystal Structures: The Close-Packing Principle Revisited.* MIF++ Seminar, Materials Innovation Factory, University of Liverpool, UK, October 7
- **2024**: *Geometry-Informed Optimization for Targeted Material Design: From Statistical Manifolds to Crystalline Frameworks.* PDRA – DS Seminar Series, Centre for Doctoral Training in Distributed Algorithms, University of Liverpool, UK, May 9
- **2023**: *Maximally Dense Crystallographic Symmetry Group Packings through Entropic Trust Region: An Information Geometric Perspective.*
  - Theory Cluster Meeting, Brunner Lecture Theater, University of Liverpool, UK, October 12
  - Applied Geometry and Topology Network Meeting, Materials Innovation Factory, University of Liverpool, UK, September 21
- **2023**: *Symmetries of Maximally Dense Plane Group Packings of Regular Convex Polygons.* Mathematics and Computer Science for Materials Innovation 2023 (MACSMIN), Materials Innovation Factory, University of Liverpool, UK, May 22–26

Internal Seminar Talks

- **2025**: *Aspects of Uncertainty Quantification in Materials Discovery. AIC Group Meeting Knowledge Bites, Department of Chemistry, University of Liverpool, September 22*

Poster Presentations

- **2025**: *Geometric Modeling in the Prediction of Molecular Crystal Structures: The Close-Packing Principle Revisited.* 7th International Conference on Geometric Science of Information (GSI'25), Le Grand Large, Palais des Congrès, Saint Malo, France, October 29-31
- **2024**: *Towards Efficient Ground State Prediction of Organic Molecular Systems via Integration of Geometric Inductive Biases.* CaLISTA Workshop on Geometry-Informed Machine Learning, Mines Paris, France, September 2–5
- **2024**: *Geometry-Informed Programming: From Statistical Manifolds to Hard Packings of van der Waals Models.* Crystal Engineering (Gordon Research Conference), Maine, USA, June 23–27
- **2023**: *Geometry of the Entropic Trust Region for Maximally Dense Crystallographic Symmetry Group Packings.* 6th International Conference on Geometric Science of Information (GSI'23), Le Grand Large, Palais des Congrès, Saint Malo, France, August 30 – September 1
- **2022**: *Geometry of the n-Torus Entropic Trust Region Packing Algorithm.* Conference on the Mathematics of Complex Data, KTH Royal Institute of Technology, Stockholm, Sweden, June 13–16

Awards and Honors

- **2025**: The Leverhulme Research Centre for Functional Materials Design Training Fund Award.
  - Project title: *In-person participation in the ICERM "Matroids, Rigidity, and Algebraic Statistics" and "Geometry of Materials" workshops.*
  - **Awarded Amount**: £4,680
- **2024**: COST Action CA21109 — Cartan Geometry, Lie, Integrable Systems, Quantum Group Theories for Applications (CaLISTA) Short-Term Scientific Mission Grant. Joint with Roland Púček (University of Jena).

    - Project title: *Integral Formulae for Solutions of PDEs with Constant Coefficients and Their Integrability.*
    - **Awarded Amount**: €2,000
- **2023**: COST Action CA21109 — Cartan Geometry, Lie, Integrable Systems, Quantum Group Theories for Applications (CaLISTA) Short-Term Scientific Mission Grant. Joint with Roland Púček (University of Jena).
    - Project title: *Exploring the Duality Between Geometric Networks and Stochastic Learning Machines Through the Lens of the Crystallization Conjecture.*
    - **Awarded Amount**: €2,000

Professional Memberships

- **2023–Present**: COST Action CA21109 — Cartan Geometry, Lie, Integrable Systems, Quantum Group Theories for Applications — Working Group 4 (Vision Models)

Teaching Experience

- **2024**: *Tutorial on Geometry-Informed Machine Learning for Materials Science.* Developed and delivered a tutorial for first-year Ph.D. students at the Centre for Doctoral Training in Digital and Automated Materials Chemistry, University of Liverpool, as part of the Winter School on Robotics and AI for Materials Discovery.

Professional Service

Journal Peer Review

- **2023**: Pattern Recognition (Elsevier)
- **2019**: IEEE Transactions on Neural Networks and Learning Systems

Conference and Workshop Participation

- **2**025: *Workshop on mol-CSPy - the Day group crystal structure prediction software*, School of Chemistry and Chemical Engineering, University of Southampton, United Kingdom, September 25–26
- **2**025: *Lennard-Jones Centre-CECAM Meeting 2025: From electrons to atoms to molecules and materials*, Cavendish Laboratory, Department of Physics, University of Cambridge, United Kingdom, September 1–5 (remote attendance)

- **2**025: *Geometry of Materials*, Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University , Rhode Island, April 7–11
- **2**025: *Matroids, Rigidity, and Algebraic Statistics*, Institute for Computational and Experimental Research in Mathematics (ICERM), Brown University , Rhode Island, March 17–21
- **2023**: *Training School on Cartan Geometry*, Masaryk University, Brno, Czech Republic, September 4–8

Professional Development

- **2024**: Prosper Postdoctoral Career Development Programme (2024 Cohort), University of Liverpool

Programming Experience

- MATLAB, Julia, Python, R, C++, Java, C#, Haskell, Fortran