

List of publications of Alexey V. Lyulin (h index 45, ~6000 citations)

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Proceedings

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3. A.V. Lyulin, M.A.J. Michels, *Computer Simulation Study of Correlated Segmental Dynamics in Isotropic and Deformed Atactic Polystyrene*, 12th Int. Conf. on "Deformation, Yield and Fracture of Polymers", Cambridge, 7-10 April, 2003.
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7. S. Lyulin, A. Darinskii, A. V. Lyulin, *Internal Dynamics of Dendrimer – Linear Polyelectrolyte Complexes*, European Polymer Congress, Portoroz, Slovenia, 2007.
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9. A.V. Lyulin, M.A.J. Michels, *Direct Atomistic Modelling of Deformed Polymer Glasses*, XVth International Congress on Rheology, August 2008, Monterey, USA

10. Alexey V. Lyulin, Dmitri Hudzinsky, Eric Janiaud and Antoine Chateauinois
Rejuvenation Effects in Polymer Glassy Dynamics
5th International Multiscale Materials Modelling Conference, 4-8 October 2010, Freiburg, Germany, proceedings, p. 222-225.
11. Andrea Muntean, Alexey V. Lyulin,
Molecular-dynamics simulations of oxidation effects on properties of polystyrene surfaces
5th International Multiscale Materials Modelling Conference, 4-8 October 2010, Freiburg, Germany, proceedings, p. 623-626.
12. C. Batistakis, M.A.J. Michels and Alexey V. Lyulin
Molecular-Dynamics Simulations of Mechanical Reinforcement in Filled Elastomers
Eds: DAmore, A, Acierno, D., Grassia, L., 7th International Conference on Times Of Polymers and Composites (TOP), June 22-26, 2014, Ischia, Italy
AIP Conference Proceedings, 1599, 62, 2014
13. Soumyadipta Sengupta, Giorgos Kritikos, Konstantinos Karatasos, Arun Venkatnathan, Rakesh Pant, Pavel Komarov and Alexey V. Lyulin
Novel Polyelectrolyte Membranes for Fuel and Flow Batteries: Insights from Simulations
IX INTERNATIONAL CONFERENCE "TIMES OF POLYMERS AND COMPOSITES", June 17-21, **2018** Ischia , Italy.
14. L.A. van Goor, D. Jafari, H. Lee, A.V. Lyulin, W.W. Wits and B.J. Geurts, *Multiscale Modeling of Heat Transfer in Graphene-Copper Nanocomposites*, ECCOMAS Thematic Conference: Computational Modeling of Complex Materials Across the Scales, May 13-16, **2025**, Champs-sur-Marne, France

Invited Lectures

1. *Large-Scale Computer Simulation of Local Segmental Dynamics in Amorphous Atactic Polystyrene*,
Keynote lecture at the Europolymer Congress 2001, Eindhoven, July 15-20, 2001.
2. *Brownian Dynamics of Dendrimers and Hyperbranched Polymers*
Invited talk at the CECAM Workshop on "Mesoscopic Models for the Dynamics of Dead and Living Polymers", Lyon, 3-4 February, 2003.
3. *Correlated Segmental Dynamics In Isotropic and Deformed Atactic Polystyrene*,
3rd Russian Kargin Conference "Polymers-2004", Moscow, January 27 – February 1, 2004. Book of Abstracts, v.2, p.13.
4. *Molecular-dynamics Simulation of Amorphous Polymers in Isotropic State and under Uniaxial Deformation*,
Invited lecture at the 3rd Int. Conf. on BROADBAND DIELECTRIC SPECTROSCOPY AND ITS APPLICATIONS Delft, August 23-26, 2004, The Netherlands
5. *Simulating Deformed Glasses and Melts: from Simple Liquids to Polymers*,
CECAM Workshop, Lyon 12 – 14th September 2005 (organizer).
6. *Computer Simulation of Hyperbranched Polymers*,
EUPOC2006 Conference, Gargnano 7-12 May 2006.
7. *Molecular Dynamics of Polymer Glasses*,
Summer School on Mathematical Methods in Polymer and Biopolymer Physics, Petrozavodsk, Russia, 13-17 June 2006.
8. *Computer Simulation of Dendrimers and Hyperbranched Polymers*,

Summer School on Mathematical Methods in Polymer and Biopolymer Physics, Petrozavodsk, Russia, 13-17 June 2006.

9. *Hyperbranched Polymers as Novel Materials for Nanoscale Applications: Insight from Experiment, Theory and Simulations (HYPER-NANO)*, ESF/PESC Exploratory Workshop: Fodele, Crete (Greece), 25-28 May 2008 (organizer)

10. *Atomistic Modelling of Deformed Polymer Glasses*, Lorentz Workshop on Dynamic Heterogeneities in Glasses, 25/08 – 5/09 2008, Leiden.

11. *Competition of Time Scales in Short-time Response of Deformed Polymer Glasses*, 6th Int. Conference on Relaxations in Complex Systems, Rome, September 2009

12. *Scale Jumping in Computer Simulations of Polymers: from chemical scales to macromechanics and virus self-assembly* International Workshop on “Modelization and Simulation of Complex Systems” (MODELICO), Madrid, Centro de Astrobiología, November 12th, 2010.

13. Alexey Lyulin, *Confinement effects on polymer structure and glassy dynamics* Invited Paper for the March 2011 Meeting of The American Physical Society, March 21-25 2011, Dallas, Texas.

14. *Competition of time scale in short-time response of deformed polymer glasses* Invited talk at ARL meeting, Aberdeen, USA, March 2011.

15. SCM-6, Dresden, invited talk (2013)

16. 7th IDMRCS , Barcelona , invited talk (July 2013)

17. 2015 EMN International Meeting on Polymer, Orlando, Jan 7-10, FL USA.

18. 4th International Workshop on Theory and Computer Simulation of Polymers: New Developments, June 28-July 1, Halle, Germany

19. 2nd International Workshop on dendrimers and hyperbranched polymers, IRTG SoMaS, Freiburg, November 23-24, 2015.

20. 2016 EMN International Meeting on Polymer, Hong Kong, Jan 10-16, China.

21. T. Davris, A. V. Lyulin, *Molecular-dynamics simulations of crosslinking and confinement effects on structure, segmental mobility and mechanics of filled elastomers*, VIII International Conference on “Times of Polymers and Nanocomposites”, June 19-23, 2016 , Ischia, Italy

22. A. V. Lyulin, *Atomistic Simulation of Structure and Topology of Free-standing Polymer Films*, 9th Int. Symp. “Molecular Mobility and Order in Polymer Systems”, St. Petersburg, June, 2017.

23. 8th IDMRCS Symposium, Wisla, Poland, invited talk (July 2017).

24. 9th Times of Polymers and Composites (TOP) Conference, Ischia (June **2018**), invited talk.

25. Symposium on “Multiscale Mechanics of Polymers, Soft Matter and Network Materials”, 9th International Symposium on Multiscale Materials Modelling, November **2018**, Osaka (organizer).

26. SPSI-Macro-2018 International Symposium, Pune, India, 19-22 December **2018** (invited talk).

27. A. Lyulin, *Interfacial and Topological Effects on the Glass Transition in Free-standing Polymer Films*, invited talk at MPI-P (Mainz) Theoretical Colloquium, February **2018**.
28. A. Lyulin, *Computer Simulations of Novel Polyelectrolyte Membranes for Fuel Cells and Flow Batteries*, Invited Talk, EPF Congress, Heraklion, June **2019**
29. A. V. Lyulin, *In-Silico Studies of Polyelectrolyte Membranes for Flow Batteries and Fuel Cells*, 10th Int. Symp. Invited talk, "Molecular Mobility and Order in Polymer Systems", St. Petersburg, June, **2020**.
30. 10th Times of Polymers and Composites (TOP) Conference, Ischia (September **2021**), invited talk.
31. A. Lyulin, *In-Silico Studies of Polyelectrolyte Membranes for Flow Batteries and Fuel Cells*, CaSToRC Colloquium invited talk, Cyprus Institute, May **2022**
32. A. Lyulin, *Modelling of perspective polyelectrolyte membranes for flow and fuel batteries*, Invited talk, POLYCONF14, Thessaloniki, November **2023**
33. A. Lyulin, *Modelling of perspective polyelectrolyte membranes for batteries*, DAMUT Colloquium invited lecture, September **2023**
34. A. Lyulin, *Molecular-Dynamics Simulations of Hydrated Nafion Membranes*, invited talk at 9th IDMRCS Conference, Japan, August **2023**
35. A. Lyulin, "Ring juggling: how topology dictates the confined glassy dynamics of atactic polystyrene", invited talk CECAM Workshop on Ring Polymer Dynamics, Prato, June **2023**
36. Brightlands Polymer Days, Chemelot Campus, May **2024**, key-note lecture.
37. Flow4UBattery Event, Zwarte Doos, Eindhoven, April **2024**, invited talk.
38. A. Lyulin, *Designing Fast Thermal Energy Storage: Interfacial Heat Transfer in Paraffin–Graphene Composites*, invited talk at Polymers 2026: Trends, Innovation and Future, 25-28 June **2026**, Nanjing, China.