

## List of publications of Alexey V. Lyulin (h index 36, 3800 citations)

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129. S. Sengupta, A.V. Lyulin, G. Kritikos, K. Karatasos, A. Venkatnathan, R. Pant, P. Komarov, *Multiscale modelling examples: new polyelectrolyte nanocomposite membranes for perspective fuel cells and flow batteries*, in Nanocomposites, book chapter, Springer. **2020**.
130. K. Gao, H. Wan, E. Tsen, J. Liu, A. Lyulin, L. Zhang, *Unveiling the Mechanism of the Location of the Grafted Nanoparticles in Lamellar-Forming Block Copolymer*, Langmuir, 36, 194-203 **2020**.
131. C. Rafaelli, A. Bose, C.H.M.P. Vrusch, S. Ciarella, T. Davris, N.B. Tito, A.V. Lyulin, W.G. Ellenbroek, and C. Storm, *Rheology, rupture, reinforcement and reversibility: Computational approaches for dynamic network materials*. In: Advances in Polymer Science. Springer, Berlin, Heidelberg **2020**.
132. Soumyadipta Sengupta, Alexey Lyulin, *Dissipative Particle Dynamics Modelling of Polyelectrolyte Membrane-Water Interfaces*, Polymers, 12, 907 **2020**.
133. V. Sundaram, A. Lyulin, and B. Baumeijer, *Development and Testing of an All-Atom Force Field for Diketopyrrolopyrrole Polymers with Conjugated Substituents* **2020**
134. A. V. Lyulin S. Sengupta, A. Varghese, P. Komarov and A. Venkatnathan, Effect of annealing on structure and diffusion in hydrated Nafion membranes, ACS J. Appl. Polym. Mater., accepted, **2020**
135. Victor M. Nazarychev, Artyom D. Glova, Igor V. Volgin, Sergey V. Larin, Alexey V. Lyulin, Sergey V. Lyulin, Andrey A. Gurtovenko, *Evaluation of thermal conductivity of organic phase-change materials from equilibrium and non-equilibrium computer simulations: Paraffin as a test case*, **2020**

### Proceedings

1. D.B. Adolf, A.V. Lyulin, G.R. Davies, *Computer Simulation of Dendrimers and Hyperbranched Polymers*, ACS Symposium Series, 222(8), U381, 2001.
2. M.A.J. Michels, A.V. Lyulin, *Computer-Simulation Study of Bulk Atactic Polystyrene in the Vicinity of the Glass Transition*, 4<sup>th</sup> Int. Symp. "Molecular Order and Mobility in Polymer Systems", St. Petersburg, June 3-7, 2002.
3. A.V. Lyulin, M.A.J. Michels, *Computer Simulation Study of Correlated Segmental Dynamics in Isotropic and Deformed Atactic Polystyrene*, 12<sup>th</sup> Int. Conf. on "Deformation, Yield and Fracture of Polymers", Cambridge, 7-10 April, 2003.
4. A.V. Lyulin, B. Vorselaars, M.A.J. Michels,

*Molecular-dynamics simulation of amorphous polymers in the isotropic state and under uniaxial deformation*,  
CIMTEC, Sicily, 2004.

5. A. V. Lyulin,  
*Atomistic Simulation of Bulk Mechanics and Local Dynamics of Amorphous Polymers*,  
5<sup>th</sup> Int. Symp. "Molecular Mobility and Order in Polymer Systems", St. Petersburg, June, 2005.

6. I.V. Neratova, M.A. Mazo, E.F. Oleinik, N.K. Balabaev, A.V. Lyulin,  
*Computer Modelling of the Plastic Deformation for Atactic Polystyrene*,  
Tver University, 2007.

7. S. Lyulin, A. Darinskii, A. V. Lyulin,  
*Internal Dynamics of Dendrimer – Linear Polyelectrolyte Complexes*,  
European Polymer Congress, Portoroz, Slovenia, 2007.

8. S. Larin, A. Darinskii, A. V. Lyulin, S. Lyulin,  
*Dendrimer-Linear Polyelectrolyte Complexes at Low Ph Values*,  
European Polymer Congress, Portoroz, Slovenia, 2007.

9. A.V. Lyulin, M.A.J. Michels,  
*Direct Atomistic Modelling of Deformed Polymer Glasses*,  
XV<sup>th</sup> International Congress on Rheology, August 2008, Monterey, USA

10. Alexey V. Lyulin, Dmitri Hudzinsky, Eric Janiaud and Antoine Chateauminois  
*Rejuvenation Effects in Polymer Glassy Dynamics*  
5<sup>th</sup> 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*  
5<sup>th</sup> 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., 7<sup>th</sup> 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.

#### **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*,

3<sup>rd</sup> 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 3<sup>rd</sup> 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 – 14<sup>th</sup> 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*,

6<sup>th</sup> 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 12<sup>th</sup>, 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. 7<sup>th</sup> IDMRCS , Barcelona , invited talk (July 2013)

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

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

19. 2<sup>nd</sup> 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*, 9<sup>th</sup> Int. Symp. "Molecular Mobility and Order in Polymer Systems", St. Petersburg, June, 2017.
23. 8<sup>th</sup> IDMRCS Symposium, Wisla, Poland, invited talk (July 2017).
24. 9<sup>th</sup> Times of Polymers and Composites (TOP) Conference, Ischia (June **2018**), invited talk.
25. Symposium on "Multiscale Mechanics of Polymers, Soft Matter and Network Materials", 9<sup>th</sup> 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**.