Nikolaos Lempesis

Assistant Professor of Computational Chemistry

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PROFILE

My research lies at the intersection of **chemical engineering**, **computational chemistry** and **materials science**. I am well knowledgeable in multiscale simulations of complex physicochemical systems at thermodynamic equilibrium and beyond, including, but not limited to, polymer melts and nanocomposites, biomolecules and mixed hybrid organic/inorganic catalytic and photonic frameworks. I am well versed in mathematical modelling applicable in materials science for promoting sustainable chemistry, circular economy of materials, energy conversion and conservation. I am vigorously interested in conducting teaching and research in science & engineering of innovative materials, applications, and technologies to solve daily life problems, improve societal well-being and support the advancement of knowledge.

RESEARCH INTERESTS

Enthused to work on mathematical, computational and simulation sciences that translate to the cutting edge of materials research. Developing and delivering theoretical frameworks that describe the underlying structure-property-function relationships to advance novel scientific endeavors. Facilitating the fusion of theory and experimentation by intelligent and intuitive software technologies.

PERSONAL DATA

Date of birth: 28 September 1980
Place of birth: Athens, Greece
Citizenship: Greek
Marital Status: Married

POSITIONS

Current:

28/1/2025 – present
Assistant Professor (on tenure track)
Sector of Physical Chemistry
Department of Chemistry
University of Ioannina
Role: Development and application of multiscale simulation methods with practical applications in energy, environment and improvement of life quality. Conducting teaching in undergraduate and graduate courses, as well as inspiring new researchers and future thinkers.

Previous:

1/5/2021 – 31/12/2024
Research Associate
Institute of Chemical Sciences & Engineering
School of Basic Science
Swiss Federal Institute of Technology Lausanne (EPFL)
Role: Design of mixed ab initio/classical computational methods and application, adaption and extension to systems of chemical and/or biological interest

15/1/2018 – 30/4/2021
Research Associate
Department of Mechanical Engineering
School of Engineering and Architecture of Fribourg (HEIA-FR)
Role: Leading research projects; bridging the gap between academic knowledge and industrial needs through simulation and modeling

1/2/2017 – 30/6/2018
Postdoctoral Research Associate
Department of Mechanical Engineering
Swiss Federal Institute of Technology Zurich (ETH)
Role: Developing computational tools to aid material scientists in their research, discoveries and commercial activities.

1/10/2013 – 30/9/2016
Postdoctoral Research Associate
Department of Chemical Engineering
Massachusetts Institute of Technology (MIT)
Project Title: “Multiscale Theoretical Modeling of Thermoplastic Polyurethanes”

3/9/2012 – 14/9/2012
Visiting Doctoral Student
Department of Mechanical Engineering
Technische Universiteit Eindhoven (Eindhoven, Netherlands)

- Development and optimization of stochastic algorithms

1/10/2011 – 31/12/2011
Visiting Doctoral Student
Institute of Physics
Université Pierre-et-Marie-Curie UPMC (Paris, France)

- HPC-Europa2 Fellow
- Development of highly scalable simulation codes

EDUCATION

14/1/2008 – 5/6/2013
National Technical University of Athens (Athens, Greece)
Ph.D. in Materials Science

- Dissertation Title: "*Molecular simulation of glass forming materials*"
- Thesis Advisor: Professor Doros N. Theodorou
- Concentration: Computational Modeling of Polymer Mechanics

9/5/2008 – 10/11/2008
Military Service (Athens, Greece)
Fulfilled (mandatory)

- Specialization: Chemical Engineer in Greek Army

1/3/2006 – 30/11/2007
National Technical University of Athens (Athens, Greece)
M.Sc. in Materials Science

- Thesis: *"Computational study of the vitrification process by molecular simulation: the existence of inherent structures and their significance"*
- Advisor: Professor Doros N. Theodorou
- Concentration: Modeling of Polymers

10/9/2003 – 30/9/2005
Technical University of Munich (Munich, Germany)
B.Sc. in Chemical Engineering, ***GPA – 1.8/6.0***

- Direction: Bio-process engineering
- Advisor: Professor Dr. Johannes A. Lercher

- Concentration: Process Engineering and Chemical Technology

08/10/1999 – 30/11/2007
National Technical University of Athens (Athens, Greece)
B.Sc. in Chemical Engineering, ***GPA – 9.2/10***
*(**Magna Cum Laude**)*

- Direction: Materials Science
- Advisor: Professor Doros N. Theodorou
- Concentration: Thermodynamics, Solid Mechanics and Fluid Rheology

PROFESSIONAL EXPERIENCE

The Dow Chemical Company (Terneuzen, Netherlands)
Scientific Collaborator/Consultant
Feb. 2017 – Feb 2020

- Numerical modeling & simulation of thermosetting polyurethane foams
- Simulation of the free rise and mold-filling process
- Investigation of bubble size distribution and thermal properties of the foam

BASF SE (Ludwigshafen, Germany)
Scientific Collaborator/Consultant
Oct. 2013 – Sep. 2016

- Theoretical multi-scale modeling of thermoplastic polyurethanes
- Performed molecular mechanics and structural modeling
- Conducted atomistic modeling of large tensile/compressive deformation
- Coupling with micromechanical modeling and continuum scale simulations

Evonik Industries AG (Hanau, Germany)
R & D Engineering Design Intern
Nov. 2005 – Feb. 2006

- Worked in the Computer Aided Process Engineering (CAPE) department
- Performed chemical process design and optimization via ASPEN PLUS
- Dynamic simulation and optimization of a distillation column in the presence of chemical reactions

AWARDS, GRANTS AND SCHOLARSHIPS

2021	1st Prize (CHF 500) in the Polymer Replication on Nanoscale (PRN) 2021 Image contest
2012	Award from the Technical Chamber of Greece (T.E.E.) for academic achievements at NTUA
2011	HPC-Europa2 Transnational Access program fellowship to visit GENCI-CINES (Oct 1, 2011 – Dec 31, 2011) in Paris and Montpellier/France
2010	"NTUA Thomaidion award" 2010 for scientific publication on peer-reviewed journals
2010	National Strategic Reference Framework (NSRF), HERACLITUS II/ Hellenic

	Ministry of National Education and Religious Affairs: Ph.D. Scholarship Program
2008	Silver medal “Prometheus Pyrforos”, emblem of NTUA, for graduating second in rank in the year 2007
2007-2009	Scholarship of the Department of Materials Science and Engineering of the NTUA
2007-2008	Scholarship of the Bodossakis Foundation
2007	Scholarship and award by the National Scholarship Foundation of Greece (I.K.Y.) for the best effort in undergraduate studies, NTUA 2000, 2001, 2003
2003	EU Scholarship for the participation in the T.I.M.E. Double Degree Program
2000-2003	Kefalogianni award for undergraduate academic achievements at the NTUA.

BOARDS AND APPOINTMENTS

2021-present	Member of the Swiss Chemical Society (SCS) (www.scg.ch)
2020-present	Honorary Rosalind Member of London Journals Press (http://journalspress.com)
2018-present	Member of the European Materials Modeling Council (https://emmc.eu/)
2008-2013	Member of the NTUA-council of PhD students
2003-2007	Member and Fellow of the DOUBLE-DIPLOMA Top Industrial Managers of Europe (T.I.M.E.) association

COMMUNITY ENGAGEMENT

Nov 2019	Organizing Committee, 4th Plastics Update Conference, 2019, Fribourg, Switzerland
Nov 2018	Organizing Committee, 3rd Plastics Update Conference, 2018, Fribourg, Switzerland
2014-2016	Chairman, MIT 10.975 Seminar in Polymer Science and Engineering
Aug 2009	Member of the Organizing Committee, Diffusion Fundamentals III conference 2007, Athens, Greece
May 2007	Member of the Organizing Committee, Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece

PUBLICATIONS

Software

1. N. Lempesis, A. Janka, O. Gnatiuk, S. J. L. van Eijndhoven, R. J. Koopmans, “Improved wetting model for the prediction of topography and dimensionality of superomniphobic surfaces”, *Materials Cloud Archive,* **2021**, www.doi.org/10.24435/materialscloud:z5-ec

Papers

2. G. AlSabeh, V. Slama, M. Ren, M. Almalki, L. Pfeifer, D. J. Kubicki, P. Zimmermann, A. Hinderhofer, F. Faini, D. Moia, M. Othman, F. T. Eickemeyer, V. Carnevali, N. Lempesis, A. Vezzosi, F. Ansari, F. Schreiber, J. Maier, C. M. Wolff, A. Hessler-Wyser, C. Ballif, G. Grancini, U. Rothlisberger, M. Grätzel, J. V. Milić, ***Angew. Chem. Int. Ed.*** 2025, 64,

e202417432
3. Liu, Z., Lin, R., Wei, M. *et al.* All-perovskite tandem solar cells achieving >29% efficiency with improved (100) orientation in wide-bandgap perovskites. ***Nat. Mater.*** 2025, 24, 252–259
4. J. Jeong, T. Chawanpunyawat, M. Kim, V. Sláma, N. Lempesis, L. Agosta, V. Carnevali, Q. Zhang, F. T. Eickemeyer, L. Pfeifer, Y. Kim, J. W. Song, H. Lu, M. Almalki, S.-I. Mo, S. M. Zakeerudin, U. Rothlisberger, D. S. Kim, P. J. Dyson, M. Grätzel, Carbazole Treated Waterproof Perovskite Films with Improved Solar Cell Performance. ***Adv. Energy Mater.*** 2025, 15, 2401965
5. W. Luo, S. Kim, N. Lempesis, L. Merten, E. Kneschaurek, M. Dankl, V. Carnevali, L. Agosta, V. Slama, Z. VanOrman, M. Siczek, W. Bury, B. Gallant, D. J. Kubicki, M. Zalibera, L. Piveteau, M. Deconinck, L. A. Guerrero-León, A. T. Frei, P. A. Gaina, E. Carteau, P. Zimmermann, A. Hinderhofer, F. Schreiber, J. Moser, Y. Vaynzof, S. Feldmann, J.-Y. Seo, U. Rothlisberger, J. V. Milić, From Chalcogen Bonding to S–π Interactions in Hybrid Perovskite Photovoltaics. ***Adv. Sci.*** 2024, 11, 2405622
6. L. Li, M. Wei, V. Carnevali, H. Zeng, M. Zeng, R. Liu, N. Lempesis, F. T. Eickemeyer, L. Luo, L. Agosta, M. Dankl, S. M. Zakeeruddin, U. Roethlisberger, M. Grätzel, Y. Rong, X. Li, Buried-Interface Engineering Enables Efficient and 1960-Hour ISOS-L-2I Stable Inverted Perovskite Solar Cells. ***Adv. Mater.*** 2024, 36, 2303869
7. Park, S.M., Wei, M., Lempesis, N. *et al.* Low-loss contacts on textured substrates for inverted perovskite solar cells. ***Nature***, 2023, 624, 289–294
8. E. A. Alharbi, A. Krishna, N. Lempesis, M. Dankl, I. Mosquera-Lois, M. A. Hope, T. P. Baumeler, G. Kakavelakis, A. Mishra, F. Eickemeyer, O. Ouellette, T. Chawanpunyawat, A. Hagfeldt, S. M. Zakeeruddin, L. Emsley, L. Pfeifer, U. Röthlisberger and M. Grätzel, “Cooperative passivation of perovskite solar cells by alkyldimethylammonium halide amphiphiles”, ***Joule***, 2023, 7, 183-200
9. N. Lempesis, R. J. Koopmans, R. Diez-Ahedo, P. M. Kristiansen, “Extension and validation of a revised Cassie-Baxter model for tailor-made surface topography design and controlled wettability”, ***Surf. Topogr.: Metrol. Prop.***, 2021, *9*, 025021
10. N. Lempesis, A. Janka, O. Gnatiuk, S. J. L. van Eijndhoven, R. J. Koopmans, “Predicting Bio-inspired Candidate Surfaces with Superomniphobic Characteristics”, ***Surf. Topogr.: Metrol. Prop.***, 2020, *8*, 025021
11. S. Zhu, N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge, “Molecular Simulation of Thermoplastic Polyurethanes under Large Compressive Deformation” ***Macromolecules***, 2018, *51* (22), 9306-9316
12. N. Lempesis, N. Smatsi, V. G. Mavrantzas, S. E. Pratsinis, “Temperature- and pressure-induced monoclinic to orthorhombic phase transition in silicalite-1”, ***J. Phys. Chem. C***, 2018, *122*(11), 6217-6229
13. S. Zhu, N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge, “Molecular Simulation of Thermoplastic Polyurethanes under Large Tensile Deformation”, ***Macromolecules***, 2018, *51* (5), 1850-1864
14. N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge, “Atomistic Simulation of a Thermoplastic Polyurethane and Micromechanical Modeling”, ***Macromolecules***, 2017, *50*(18), 7399-7409
15. N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge, “Simulation of the structure and mechanics of crystalline 4,4’-diphenylmethane diisocyanate (MDI) with n-butanediol (BDO) as chain extender”, ***Polymer,*** 2016, *107*, 233-239
16. N. Lempesis, P. J. in ‘t Veld, G. C. Rutledge, “Atomistic simulation of the structure and mechanics of a semicrystalline polyether”, ***Macromolecules,*** 2016, *49*(15), 5714-5726
17. N. Lempesis, G. G. Vogiatzis, G. C. Boulougouris, L. C. A. van Breemen, M. Hütter, and

D. N. Theodorou, “Tracking a glassy polymer on its energy landscape in the course of elastic deformation”, ***Molecular Physics***, 2013, *111*, 3430-3441
18. N. Lempesis, G. C. Boulougouris, D. N. Theodorou, “Temporal disconnectivity of the energy landscape in glassy systems”, ***J. Chem. Phys.***, 2013, *138*, 12A545
19. N. Lempesis, D. G. Tsalikis, G. C. Boulougouris, D. N. Theodorou, “Lumping analysis for the prediction of long-time dynamics: from monomolecular reaction systems to inherent structure dynamics of glassy materials”, ***J. Chem. Phys.***, 2011, *135*, 204507
20. D. G. Tsalikis, N. Lempesis, G. C. Boulougouris, D. N. Theodorou, “Efficient parallel decomposition of dynamical sampling in glass forming materials based on an “on the fly” definition of metabasins.”, ***J. Chem. Theory Comput.***, 2010, *6*(4), 1307-1322
21. D. G. Tsalikis, N. Lempesis, G. C. Boulougouris, D. N. Theodorou, “Temperature accelerated dynamics in glass forming materials”, ***J. Phys. Chem. B***, 2010, *114*, 7844-53
22. D. G. Tsalikis, N. Lempesis, G. C. Boulougouris, D.N. Theodorou, “On the role of “inherent structures” in glass-forming materials: II. Reconstruction of the Mean Square Displacement by rigorous “lifting” of the inherent structure dynamics”, ***J. Phys. Chem. B***, 2008**,** *112*, 10628-10637
23. D. G. Tsalikis, N. Lempesis, G. C. Boulougouris, D.N. Theodorou, “On the role of "inherent structures" in glass-forming materials: I. The vitrification process”, ***J. Phys. Chem. B***, 2008**,** *112*, 10619-10627

SELECTED CONFERENCE TALKS, PAPERS AND POSTERS

1. **N. Lempesis**, A. Alexiu, U. Röthlisberger, “*Atomistic simulation of grain boundaries in metal-halide perovskites*”, 10th Annual National Centre of Competence in Research (NCCR) Molecular Ultrafast Science and Technology (MUST) Meeting, Sep 13-15 2021, Dorfstrasse 168, CH-3818, Grindelwald, Switzerland
2. **N. Lempesis**, “*Controlling wettability through modeling-based surface topography engineering*”, 7th Polymer Replication on Nanoscale (PRN) Conference, May 27-28 2021, online conference
3. **N. Lempesis**, “*Predicting Bio-inspired Surfaces*”, Swiss Plastics Expo, Halle 2, Jan 21 2020, Messe Luzern AG, Horwerstrasse 87, CH-6005 Luzern **[invited talk]**
4. **N. Lempesis**, “*Ceramic Injection Molding: A Multiscale Modeling Paradigm*”, 4th Plastics Update Conference, Nov 14 2019, School of Engineering and Architecture, Boulevard de Pérolles 80, CH-1700 Fribourg, Switzerland
5. **N. Lempesis**, “*Predicting Bio-inspired Surfaces with Superomniphobic Traits*” & “*Modeling of Ceramic Injection Molding for Medical Applications: A Multiscale Modeling Paradigm*”, ExxonMobil R&D Days, Nov 4-7 2019, ExxonMobil – European Technology Center, Hermeslaan 2, B-1831 Machelen, **[invited contribution]**
6. **N. Lempesis**, “*Understanding the Behavior and Tailor-making the Properties of Thermoplastic Polyurethanes: A Multiscale Modeling Paradigm*”, 3rd Plastics Update Conference, Nov 15 2018, School of Engineering and Architecture, Boulevard de Pérolles 80, CH-1700 Fribourg, Switzerland **[invited talk]**
7. **N. Lempesis**, “*Bio-inspired wetting models with superomniphobic traits*”, IMX talk, July 2018, Institute of Materials, Ecole Polytechnique Federale de Lausanne (EPFL), Route Cantonale, CH-1015 Lausanne, Switzerland **[invited talk]**
8. **N. Lempesis**, “*Mechanics of composite materials from its constituent parts: A simulation study*”, NORA Advanced Composites Group Meeting, Jan 14 2016, Harvard Pierce Hall Rm 213, 29 Oxford Street, Cambridge MA 02138, USA **[invited talk]**
9. **N. Lempesis**, P. J. in ‘t Veld, G. C. Rutledge, “*Atomistic simulation of the structure and*

mechanics of semicrystalline and heterogeneous polymer systems", 2015 AIChE Annual Meeting, November 10 2015, Salt Lake City, Utah, USA

10. **N. Lempesis**, "*Multiscale modelling of composite polymeric materials*", NORA Meets BASF Challenges, Nov 4-5 2015, Norton Woods Conference Center at the American Academy of Arts & Sciences, 136 Irving Street, Cambridge, MA 02138, USA
11. **N. Lempesis**, P. J. in 't Veld, G. C. Rutledge, "*Atomistic simulation of a semicrystalline polyether*", 7th International Workshop and Summer School on Nonequilibrium Thermodynamics, July 2015, Hilvarenbeek, the Netherlands
12. **N. Lempesis**, "*Simulation study on the mechanical behavior of heterogeneous materials*", NORA All Projects Day, May 5 1015, Harvard School of Engineering & Applied Sciences, 20 University Road, Cambridge MA 02138, USA **[invited talk]**
13. **N. Lempesis**, "*Atomistic simulations of a common thermoplastic polyurethane*" NORA Advanced Composites Group Meeting, Jan 22 2015, MIT, 55 Massachusetts Avenue, Cambridge, MA USA **[invited talk]**
14. **N. Lempesis**, "*Atomistic simulation of the mechanics of composite materials*", NORA Advanced Composites Group Meeting, Nov 19 2014, Harvard Pierce Hall Rm 213, 29 Oxford Street, Cambridge MA 02138, USA **[invited talk]**
15. **N. Lempesis**, "*Atomistic simulation of the structure and mechanics of a polyether*", Advanced Composites Meeting, Sep 16 2014, Umass Amherst, MA USA **[invited talk]**
16. **N. Lempesis**, "*Atomistic modelling of heterogeneous composite materials*", Advanced Composites Retreat, June 29 – July 1, Woodstock Inn, Woodstock Vermont, USA
17. **N. Lempesis**, "*Theoretical Multiscale Modelling of thermoplastic Polyurethanes*", May 28 2014 NORA All Project Day, MIT Media Lab, Cambridge MA, USA **[invited talk]**
18. N. Lempesis, G. C. Boulougouris, **D. N. Theodorou**, "*Energy landscape analysis of atomic and polymer glasses"*, September 19th-21st 2012, Mainz Germany
19. N. Lempesis, G. C. Boulougouris, **D. N. Theodorou**, "*Tracking the Dynamics of Systems Evolving through Infrequent Transitions in a Network of Discrete States*", IAS Series 10 Hierarchical Methods for Dynamics in Complex Molecular Systems Lecture Notes, IAS Winter School, 5-9 March 2012, Jülich, Germany edited by J. Grotendorst, G. Sutmann, G. Gompper, D. Marx (2012)
20. D. Tsalikis, **N. Lempesis**, G. C. Boulougouris, D. N. Theodorou , "Energy Landscape–Based Study of Atomic Displacements in Glass Forming Materials*", Special Issue "Diffusion Fundamentals III" ,**11** (2009) 65, pp 1-2*
21. D. Tsalikis, N. Lempesis, G. C. Boulougouris, **D. N. Theodorou**. "*On the role of inherent structure dynamics in glass forming materials*", AIChE Annual Meeting, Philadelphia, PA November 16-21, 2008

LANGUAGES

- **Greek:** (native speaker)
- **English:** Fluent (C2)
- **German:** Advanced (C1)
- **French:** Intermediate (B1)

REVIEWER OF SCIENTIFIC JOURNALS

Reviewer of manuscripts submitted for consideration for publication in:

- **Nature**
- **Macromolecules**
- **The Journal of Physical Chemistry B**
- **The Journal of Physical Chemistry C**
- **The Journal of Chemical Physics**
- **Polymers**
- **Molecular Physics**
- **Sensors**
- **Powder Technology**