

## Curriculum Vitae

### Nikolaos I. Lempesis

**Home:** Fichtenstrasse 28, 8032 Zurich, Switzerland

**Work:** Department of Mechanical and Process Engineering  
Eidgenössische Technische Hochschule (ETH), Room ML – F25  
Sonneggstrasse 3, 8092 Zurich, Switzerland

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#### RESEARCH INTERESTS

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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

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

#### POSITIONS

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##### Current:

Feb 2017 –

Senior Research Associate

Swiss Federal Institute of Technology (ETH)

**Role:** Developing computational tools to aid material scientists in their research, discoveries and commercial activities.

##### Previous:

Oct 2013 – Jan 2017

Postdoctoral Research Associate in the Rutledge Group  
Massachusetts Institute of Technology (MIT)

**Project Title:** “Multi-scale Theoretical Modeling of Thermoplastic Polyurethanes”

## EDUCATION

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Feb 2009 – Sep 2013: Doctor of Philosophy student in Chemical Engineering and Material Science, NTUA, Athens, Greece

**Thesis Advisor:** Professor Doros N. Theodorou

**Dissertation Title:** “Molecular simulation of glass forming materials”

Mar 2008 – Nov 2008: Military Service (fulfilled)

2000-2007 Diploma and Masters in Chemical Engineering in direction of Materials Science, NTUA, Athens, Greece

**Title:** “Computational study of the vitrification process by molecular simulation: the existence of inherent structures and their significance.”

(Graduation with honors, Magna Cum Laude, grade: 9.2/10)

2003-2007 Diploma in Chemical Engineering in direction Biotechnology participating in the Top Industrial Managers of Europe (T.I.M.E.) double-degree program supported by European Union, TUM, Munich, Germany  
(Graduation grade: 1.9)

## INDUSTRIAL EXPERIENCE

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2013-now **Scientific Collaborator:** BASF SE: Materials and Systems Research, Materials Modelling Group, 38 Carl-Bosch street, Ludwigshafen D-67056, Germany, Project title: “Multi-scale theoretical modeling of thermoplastic polyurethanes” funded by the chemical company BASF SE

2005-2006 **Internship:** Degussa AG: Computer Aided Process Engineering (CAPE) department.

Project title: Dynamic simulation and optimization of a distillation column in the presence of a chemical reaction under use of the Aspen process simulation package. Rodenbacher Chaussee 4, D-63457 Hanau-Wolfgang, Germany

## AWARDS, GRANTS, PROPOSALS AND SCHOLARSHIPS

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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-Montpellier/France

2010 “NTUA Thomaidion award” 2010 for scientific publication on peer-reviewed journals

2010 National Strategic Reference Framework (NSRF), Enhancement of research man power through the implementation of thesis – HERACLITUS II/ Hellenic Ministry of National Education and Religious Affairs: PhD scholarship (Sep 1, 2010 – Aug 31, 2013) for the project entitled “Molecular simulations of glass

- forming materials”
- 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 for the academic years 2000,2001 and 2003 offered by the National Scholarship Foundation of Greece (I.K.Y.) for the best effort during the first three academic years at NTUA.
- 2003 EU Scholarship for the participation to the T.I.M.E. Double Degree Program
- 2000-2003 Kefalogianni award for academic achievements at the NTUA.

## BOARDS AND APPOINTMENTS

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- 2008-now Member of the NTUA-council of PhD students
- 2003-now Member of the Top Industrial Managers of Europe (T.I.M.E.) association

## COMMUNITY ENGAGEMENT

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- 2014-now Committee Chairman of the MIT 10.975 Seminar in Polymer Science and Engineering
- Aug 2009 Member of the Organizing Committee, Diffusion Fundamentals III conference, Athens, Greece
- May 2007 Member of the International Organizing Committee, Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007), Hersonissos, Crete, Greece

## SUPERVISION

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- 2015-now Mentor of multiple undergraduate students in the context of MIT's Undergraduate Research Opportunities Program (UROP). Project title: “Molecular analysis of the structure of a thermoplastic polyurethane (TPU)”
- 2014-now Mentoring and supervising of numerous PhD students in the field of materials science and computational simulation of mater.
- 2011-2012 Supervising and mentoring Diploma Thesis and Masters students in the Computational Materials Science and Engineering Group, School of Chemical Engineering, NTUA

## TAUGHT COURSES – SEMINARS

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- Jun 16 – Jul 16 Introduction to debugging techniques and software tools, MIT
- Jun 15 – Jul 15 Introduction to parallel programming, MIT
- Jun 14 – Jul 14 Introduction to Unix/Linux operating systems, MIT
- Jan 08 – 2013 Physical Chemistry II: States of matter – Phase Equilibria, NTUA
- Jan 08 – 2013 Tutor and supervisor, Laboratory experiments of core undergraduate course

## SOFTWARE & CODING SKILLS

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**Administration:** Workstations, clusters (administration and maintenance)

**Operating Systems:** MS-Windows (all), Linux, Unix, Mac OS

**Programming Languages:** Fortran (all), C, Python

**Parallel Computing:** MPI, Open-MP

**Modelling and Mathematical Software:** Wolfram Mathematica, Matlab, Aspen, Scienomics  
MAPS, Materials Studio, LAMMPS, GROMACS, EMC, Totalview

## PUBLICATIONS

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1. 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  
[Impact factor 5.835, Citations 1]
2. 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  
[Impact factor 3.684, Citations 3]
3. 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  
[Impact factor 5.835, Citations 3]
4. 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  
[Impact factor 1.720, Citations 3]
5. N. Lempesis, G. C. Boulougouris, D. N. Theodorou, "Temporal disconnectivity of the energy landscape in glassy systems", *J. Chem. Phys.*, **2013**, 138, 12A545  
[Impact factor 3.017, Citations 3]
6. N. Lempesis, 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  
[Impact factor 3.017, Citations 6]
7. D. 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  
[Impact factor 5.498, Citations 9]
8. D. Tsalikis, N. Lempesis, G. C. Boulougouris, D. N. Theodorou, "Temperature accelerated dynamics in glass forming materials", *J. Phys. Chem. B*, **2010**, 114, 7844-53  
[Impact factor 3.302, Citations 5]
9. D. 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  
[Impact factor 3.302, Citations 7]

10. D. 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  
[Impact factor 3.302, Citations 14]

## CONFERENCE TALKS, PAPERS AND POSTERS

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1. **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
2. **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<sup>th</sup> 2015, Salt Lake City, Utah, USA
3. **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
4. **N. Lempesis**, P. J. in 't Veld, G. C. Rutledge, "*Atomistic simulation of a semicrystalline polyether*", 7<sup>th</sup> International Workshop and Summer School on Nonequilibrium Thermodynamics, July 2015, Hilvarenbeek, the Netherlands
5. **N. Lempesis**, "*Simulation study on the mechanical behavior of heterogeneous materials*", NORA All Projects Day, May 5 2015, Harvard School of Engineering & Applied Sciences, 20 University Road, Cambridge MA 02138, USA
6. **N. Lempesis**, "*Atomistic simulations of a common thermoplastic polyurethane*" NORA Advanced Composites Group Meeting, Jan 22 2015, MIT, 55 Massachusetts Avenue, Cambridge, MA USA
7. **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
8. **N. Lempesis**, "*Atomistic simulation of the structure and mechanics of a polyether*", Advanced Composites Meeting, Sep 16 2014, Umass Amherst, MA USA
9. **N. Lempesis**, "*Atomistic modelling of heterogeneous composite materials*", Advanced Composites Retreat, June 29 – July 1, Woodstock Inn, Woodstock Vermont, USA
10. **N. Lempesis**, "*Theoretical Multiscale Modelling of thermoplastic Polyurethanes*", May 28 2014 NORA All Project Day, MIT Media Lab, Cambridge MA, USA
11. N. Lempesis, G. C. Boulougouris, **D. N. Theodorou**, "*Energy landscape analysis of atomic and polymer glasses*", September 19<sup>th</sup>-21<sup>st</sup> 2012, Mainz Germany
12. 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)
13. 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
14. 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

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Greek, English, German

## OTHER INTERESTS

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Sports, Music, Travel

## REFEREES

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Prof. Doros N. Theodorou

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