# Curriculum Vitae: Dr. Loukas D. Peristeras

# Chemical engineer, PhD

## Current

Researcher C, Molecular Thermodynamics and Modelling of Materials Laboratory (MTMML), Institute of Nanoscience and Nanotechnology, NCSR "Demokritos"

## Contact

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## Scientific Resume

My research activity focus in the prediction of macroscopic properties of materials with complex chemical constitution and molecular architecture using molecular simulations and thermodynamic modeling. Developing powerful algorithms and methods for the creation of initial configurations and the thermodynamic equilibration of complex molecular systems in various environments is the core of my work. Moreover, I am interested to promote and facilitate the application of these methods by developing computational end-user tools for both academic and industry research and development activities.

## Personal

Year of Birth: 1970

Citizenship: Greek

Languages: English, Greek

Leisure activities: Literature reading, cinema and theater, walking

## Education

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| 2003: | **PhD in Chemistry** (Molecular Modeling of Materials)  PhD thesis: “*Effect of Molecular Architecture on the Thermodynamics Properties of Polymer Blends Using Molecular Simulation Methods*”  Department of Chemistry, National and Kapodistrian University of Athens |
| 2000: | **Masters Degree in Polymer Science**  Dissertation topic: “*Modeling of Systems of Well Defined Linear and Branched Polymers Using Molecular Mechanics Method*”  Department of Chemistry, National and Kapodistrian University of Athens, Postgraduate program: “Polymer Science and its Applications” |
| 1996: | **Degree in Chemical Engineering**  Diploma thesis: ‘‘*Mathematical Modeling of non Ideal Flow in a Membrane Reactor of Industrial Scale*’’  National Technical University of Athens |

## Professional Activity

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| 2016- current: | **Researcher** at Molecular Thermodynamics and Modelling of Materials Laboratory, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos" |
| 2014-2016: | **Special research scientist** at Molecular Thermodynamics and Modelling of Materials Laboratory, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos" |
| 2006-2014: | **Senior research scientist** at Scienomics SARL, France |
| 2003-2005: | **Postdoctoral researcher** at Computational Materials Science and Engineering group (COMSE) of National Technical University of Athens (NTUA) |
| 2001-2003: | **Postgraduate researcher** in the Molecular Modeling of Materials Laboratory (MMML) of NRCPS "Demokritos" |
| 2000-2001: | **Research assistant** in MMML of NRCPS "Demokritos" |
| 1998-2003: | **System administrator** of computing resources of the MTMML at NRCPS "Demokritos" |
| 1995: | **Laboratory assistant** in "Computing Languages – Fortran" course at the Department of Chemical Engineering of the NTUA |
| 1994: | **Assistant engineer** in the waste water plant of Kalamata (practical exercise for 3 months) |

## Selected Projects

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| 1. “*Thermodynamic and Phase Equilibrium Properties of Polymer Blends from Molecular Simulation, Macroscopic Modelling, and Experimental Measurements*” Funding: Greek Secretariat of Research and Technology (PENED) Role: research assistant |
| 2. “Novel Membrane Materials and Membranes for Separation of  Hydrocarbons in Natural and Petroleum Gas” Funding: NATO Science for Peace, Greek Secretariat of Research and Technology Role: postgraduate researcher |
| 3. "Computational Study of Physical Ageing and Plastic Deformation in Glassy Materials" Funding: Greek ministry of National Education and Religion (PYTHAGORAS) Role: postdoctoral researcher |
| 4. “Amorphous Builder” Funding: Scienomics SARL Role: project scientific and technical design, project implementation |
| 5. “Novel Ionic Liquid and Supported Ionic Liquid Solvents for Reversible Capture of CO2 (IOLICAP)” Funding: EU FP7 Role: proposal design and preparation for Scienomics SARL. |
| 6. “Chameleon” Funding: Consortium of private investors Role: proposal preparation, scientific and technical design |
| 7. “Techno-economic Assessment of CO2 Quality Effect on Capture, Transport and Storage (CO2QUEST)” Funding: EU FP7 Role: special research scientist |
| 8. “ShaleXEnvironmentT (No: 640979)” Funding: EU H2020 Role: Special research scientist |
| 9. “Coarse grain modelling of polysaccharides-clay nanomaterials” Funding: Stavros Niarchos Foundation (SNF), Scienomics S.A.R.L Role: Research supervisor |
| 10. “Hierarchical modeling for the optimal design of personal hygiene products (HygiMod)” (MIS 5047819) Funding: ΓΓΕΤ, ΕΣΠΑ 2014-2020 / ΕΒΔΜ Role: Principal investigator |

## Publications List

28. Papavasileiou, K.D., Peristeras, L.D., Bick, A., Economou, I.G. Molecular Dynamics Simulation of the *n* -Octacosane–Water Mixture Confined in Graphene Mesopores: Comparison of Atomistic and Coarse-Grained Calculations and the Effect of Catalyst Nanoparticle, Energy Fuels. 35 (2021) 4313–4332. <https://doi.org/10.1021/acs.energyfuels.0c04151>.

27. Tsourtou, F.D. , Peristeras L.D., Apostolov, R., Mavrantzas, V.G. Molecular Dynamics Simulation of Amorphous Poly(3-hexylthiophene), Macromolecules. 53 (2020) 7810–7824. <https://doi.org/10.1021/acs.macromol.0c00454>.

26. Papavasileiou, K.D., Peristeras, L.D., Chen, J., van der Laan, G.P., Rudra, I., Kalantar, A., Economou, I.G. Molecular dynamics simulation of the n-octacosane-water mixture confined in hydrophilic and hydrophobic mesopores: The effect of oxygenates, Fluid Phase Equilibria. 526 (2020) 112816. <https://doi.org/10.1016/j.fluid.2020.112816>.

25. Nikolaidis, I.K., Boulougouris, G.C., Peristeras, L.D., Economou, I.G. Construction of phase envelopes for binary and multicomponent mixtures with Euler-Newton predictor-corrector methods. *Fluid Phase Equilibria* **2020**, 505, 112338. <https://doi.org/10.1016/j.fluid.2019.112338>

24. Nikolaidis, I.K., Boulougouris, G.C., Peristeras, L.D., Economou, I.G. Efficient and robust methods for direct saturation point calculations. *Fluid Phase Equilibria* **2019**, 500, 112242. <https://doi.org/10.1016/j.fluid.2019.112242>

23. Papavasileiou, K.D., Peristeras, L.D., Bick, A., Economou, I.G. Molecular Dynamics Simulation of Pure *n* -Alkanes and Their Mixtures at Elevated Temperatures Using Atomistic and Coarse-Grained Force Fields. *J. Phys. Chem. B* **2019**, 123, 6229–6243. <https://doi.org/10.1021/acs.jpcb.9b02840>

22. Alexiadis, O., Cheimarios, N., Peristeras, L.D., Bick, A., Mavrantzas, V.G., Theodorou, D.N., Hill, J., Krokidis, X. Chameleon: A generalized, connectivity altering software for tackling properties of realistic polymer systems. *WIREs Comput Mol Sci* **2019**, e1414. <https://doi.org/10.1002/wcms.1414>

21. Tsourtou, F. D.; Peroukidis, S. D.; Peristeras, L. D.; Mavrantzas, V. G. Monte Carlo Algorithm Based on Internal Bridging Moves for the Atomistic Simulation of Thiophene Oligomers and Polymers. *Macromolecules* **2018**, *51* (21), 8406–8423. https://doi.org/[10.1021/acs.macromol.8b01344](https://doi.org/10.1021/acs.macromol.8b01344).

20. Tsalikis, D. G.; Alatas, P. V.; Peristeras, L. D.; Mavrantzas, V. G. Scaling Laws for the Conformation and Viscosity of Ring Polymers in the Crossover Region around Me from Detailed Molecular Dynamics Simulations. *ACS Macro Lett.* **2018**, *7* (8), 916–920. https://doi.org/[10.1021/acsmacrolett.8b00437](https://doi.org/10.1021/acsmacrolett.8b00437).

19. Papavasileiou, K. D.; Michalis, V. K.; Peristeras, L. D.; Vasileiadis, M.; Striolo, A.; Economou, I. G. Molecular Dynamics Simulation of Water-Based Fracturing Fluids in Kaolinite Slit Pores. *The Journal of Physical Chemistry C* **2018**, *122* (30), 17170–17183. https://doi.org/[10.1021/acs.jpcc.8b03552](https://doi.org/10.1021/acs.jpcc.8b03552).

18. Vasileiadis, M.; Peristeras, L. D.; Papavasileiou, K. D.; Economou, I. G. Transport Properties of Shale Gas in Relation to Kerogen Porosity. *The Journal of Physical Chemistry C* **2018**. https://doi.org/[10.1021/acs.jpcc.8b00162](https://doi.org/10.1021/acs.jpcc.8b00162).

17. Vasileiadis, M.; Peristeras, L. D.; Papavasileiou, K. D.; Economou, I. G. Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization. *Energy & Fuels* **2017**, *31* (6), 6004–6018. https://doi.org/[10.1021/acs.energyfuels.7b00626](https://doi.org/10.1021/acs.energyfuels.7b00626).

16. Takis, P. G., Papavasileiou, K. D.; Peristeras, L. D.; Boulougouris, G. C.; Melissas, V. S.; Troganis, A. N., Unscrambling micro-solvation of –COOH and –NH groups in neat dimethyl sulfoxide: insights from 1H-NMR spectroscopy and computational studies .Phys. Chem. Chem. Phys. **2017**, 19 (21), 13710–13722. 10.1039/C7CP01592E

15. Papavasileiou, K. D., Makrodimitri, Z. A., Peristeras, L. D., Chen, J., van der Laan, G. P., Rudra, I., Economou, I. G.. Molecular Simulation of n-Octacosane–Water Mixture in Titania Nanopores at Elevated Temperature and Pressure. *The Journal of Physical Chemistry C* **2016**. 10.1021/acs.jpcc.6b07226.

14. Porter, R. T. J.; Mahgerefteh, H.; Brown, S.; Martynov, S.; Collard, A.; Woolley, R. M.; Fairweather, M.; Falle, S. A. E. G.; Wareing, C. J.; Nikolaidis, I. K.; Boulougouris, G. C.; Peristeras, L. D**.**; Tsangaris, D. M.; Economou, I. G.; Salvador, C.; Zanganeh, K.; Wigston, A.; Najafali, J. N.; Shafeen, A.; Beigzadeh, A.; Farret, R.; Gombert, P.; Hebrard, J.; Proust, C.; Ceroni, A.; Flauw, Y.; Zhang, Y.; Chen, S.; Yu, J.; Talemi, R. H.; Bensabat, J.; Wolf, J. L.; Rebscher, D.; Niemi, A.; Jung, B.; Dowell, N. M.; Shah, N.; Kolster, C.; Mechleri, E.; Krevor, S., Techno-economic assessment of CO2 quality effect on its storage and transport: CO2QUEST. *International Journal of Greenhouse Gas Control* **2016**. doi: 10.1016/j.ijggc.2016.08.011.

13. Brown, S.; Peristeras, L. D**.**; Martynov, S.; Porter, R. T. J.; Mahgerefteh, H.; Nikolaidis, I. K.; Boulougouris, G. C.; Tsangaris, D. M.; Economou, I. G., Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures. *Computers & Chemical Engineering* **2016**. doi: 10.1016/j.compchemeng.2016.09.005.

12. Nikolaidis, I. K.; Boulougouris, G. C.; Peristeras, L. D.; Economou, I. G., Equation-of-State Modeling of Solid–Liquid–Gas Equilibrium of CO2 Binary Mixtures. *Industrial & Engineering Chemistry Research* **2016,** *55* (21), 6213-6226.

11. Nikolaidis, I. K.; Economou, I. G.; Boulougouris, G. C.; Peristeras, L. D., Calculation of the phase envelope of multicomponent mixtures with the bead spring method. *AIChE Journal* **2016,** *62* (3), 868-879.

10. Zubeir, L. F.; Rocha, M. A. A.; Vergadou, N.; Weggemans, W. M. A.; Peristeras, L. D**.**; Schulz, P. S.; Economou, I. G.; Kroon, M. C., Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation. *Phys. Chem. Chem. Phys.* **2016,** *18* (33), 23121-23138.

9. Tzoupis, H.; Leonis, G.; Avramopoulos, A.; Reis, H.; Czyżnikowska, Ż.; Zerva, S.; Vergadou, N.; Peristeras, L. D**.**; Papavasileiou, K. D.; Alexis, M. N.; Mavromoustakos, T.; Papadopoulos, M. G., Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays. *Journal of Molecular Graphics and Modelling* **2015,** *62*, 138-149.

8. Takis, P. G.; Papavasileiou, K. D.; Peristeras, L. D.; Melissas, V. S.; Troganis, A. N., Probing micro-solvation in “numbers”: the case of neutral dipeptides in water. *Physical Chemistry Chemical Physics* **2013,** *15* (19), 7354.

7. Lithoxoos, G. P.; Peristeras, L. D.; Boulougouris, G. C.; Economou, I. G., Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon. *Molecular Physics* **2012,** *110* (11-12), 1153-1160.

6. Lithoxoos, G. P.; Labropoulos, A.; Peristeras, L. D.; Kanellopoulos, N.; Samios, J.; Economou, I. G., Adsorption of N2, CH4, CO and CO2 gases in single walled carbon nanotubes: A combined experimental and Monte Carlo molecular simulation study. *The Journal of Supercritical Fluids* **2010,** *55* (2), 510-523.

5. Boulougouris, G. C.; Peristeras, L. D.; Economou, I. G.; Theodorou, D. N., Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations. *The Journal of Supercritical Fluids* **2010,** *55* (2), 503-509.

4. Ramos, J.; Peristeras, L. D.; Theodorou, D. N., Monte Carlo simulation of short chain branched polyolefins in the molten state. *Macromolecules* **2007,** *40* (26), 9640-9650.

3. Rissanou, A. N.; Peristeras, L. D.; Economou, I. G., Calculation of the effect of macromolecular architecture on structure and thermodynamic properties of linear–tri-arm polyethylene blends from Monte Carlo simulation. *Polymer* **2007,** *48* (13), 3883-3892.

2. Peristeras, L. D.; Rissanou, A. N.; Economou, I. G.; Theodorou, D. N., Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends. *Macromolecules* **2007,** *40* (8), 2904-2914.

1. Peristeras, L. D.; Economou, I. G.; Theodorou, D. N., Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves. *Macromolecules* **2005,** *38* (2), 386-397.

## Chapters in Books

1. Papavasileiou, K.D., Vasileiadis, M., Michalis, V.K., Peristeras, L.D., Economou, I.G. Multi-Scale Models for the Prediction of Microscopic Structure and Physical Properties of Chemical Systems Related to Natural Gas Technology, in: Natural Gas Processing from Midstream to Downstream. John Wiley & Sons , **2018**, Ltd, Chichester, UK, pp. 463–497. <https://doi.org/10.1002/9781119269618.ch18>

## Conferences

1. K.D. Papavasileiou, V.K. Michalis, L.D. Peristeras, M. Vasileiadis, A. Striolo, I.G. Economou “Water-based fracturing fluids in kaolinite slit pores: a molecular dynamics study on component distribution and mobility”, ESAT 2018, Prague, Czech Republic, (2018).
2. M. Vasileiadis, L.D. Peristeras, K.D. Papavasileiou, I.G. Economou “Transport of gases confined in kerogen: Diffusion paths, diffusion coefficients and permeability”. ESAT 2017, Bucharest, Romania (2017).
3. I.G. Economou, K.D. Papavasileiou, L.D. Peristeras, G. Van Der Laan, A. Kalantar “*Accurate prediction of physical properties for the Gas-To-Liquid process based on molecular simulation methods*”, Thermodynamics 2017, Endiburgh, Scotland (2017).
4. I.K. Nikolaidis, G.C. Boulougouris, L.D. Peristeras, I.G. Economou “*Thermodynamic Models for Solid – Liquid – Gas Equilibrium of CO2 mixtures*”, AIChE Annual Meeting, USA (2016).
5. P.G. Takis, K.D. Papavasileiou, L.D. Peristeras, C.G. Boulougouris, V.S. Melissas, A.N. Troganis “Exploring the interaction of DMSO with organic molecules of biologican interest – combing the experiment with molecular simulations”, 22th Panhellenic Conference in Chemistry, Thessaloniki, Greece (2016).
6. A. Bick, L.D. Peristeras, D.G. Tsalikis, V.G. Mavrantzas, E. Amanatides and D. Mataras, “Multiscale modeling of PECVD generated Silicon films with Kinetic Monte Carlo and LAMMPS molecular dynamics”, LAMMPS workshop and symposium, New Mexico, USA (2013).
7. Ν.Ι. Diamantonis, G. Boulougouris, D.M. Tsangaris, I.G. Economou, L.D. Peristeras, S. Martynov and H. Mahgerefteh, “CO2 Mixture Properties Using Equations of State and Molecular Simulations”, Workshop on Industrial Use of Molecular Thermodynamics (InMoTher), Lyon, France (2012).
8. G.C. Boulougouris, L.D. Peristeras, I.G. Economou and D.N. Theodorou “Bridging length scale in fluid phase equilibrium via histogram reweighting of Gibbs ensemble monte carlo simulations”, 7 GRACM-12, 2011, Athens, Greece (2011).
9. N. Diamantonis, T. Spyriouni, G.Boulougouris, L. Peristeras, D.M Tsangaris and I.G. Economou, "Prediction and regression of CO2 physical properties from equations of state and molecular simulation", Thermodynamics 2011, , Athens, Greece (2001).
10. G.P. Lithoxoos, L.D. Peristeras, G. Boulougouris and I.G. Economou, "Adsorption of CO2, CO, CH4, H2S Gases in Activated Graphite via Monte Carlo Simulation", Thermodynamics 2011, Athens, Greece (2011).
11. G.P. Lithoxoos, A. Lambropoulos, L. D. Peristeras, N. Kanellopoulos and I.G. Economou, “Experimental and Theoretical Investigation of Gas Adsorption Capacity of Pristine Single-Wall Carbon Nanotubes”, 12th International Conference on Properties & Phase Equilibria for Product and Process Design, Suzhou, China (2010).
12. G.P. Lithoxoos, A. Lambropoulos, L.D. Peristeras, N. Kannelopoulos and I.G. Economou, “Investigation of Gas Adsorption Capacity of Pristine Single-Wall Carbon Nanotubes”, International Workshop on Molecular Modeling and Simulation for Industrial Applications: Physico-Chemical Properties and Processes, Würzburg, Germany (2010).
13. G.C. Boulougouris, D.G. Tsalikis, L.D. Peristeras, and D.N. Theodorou, “Atomistic simulations of polymeric glasses over a wide time scale”, PPEPPD, Greece (2007).
14. A.N. Rissanou, L.D. Peristeras and I.G. Economou, “Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear - Tri-arm Polyethylene Blends from Monte Carlo Simulation”, 11th International Conference on Properties & Phase Equilibria for Product and Process Design, Hersonissos, Crete, Greece (2007).
15. D.G. Tsalikis, G.C. Boulougouris, L.D. Peristeras, D.N. Theodorou, “Plastic Deformation in Amorphous Polymers : a Free Energy Landscape Approach”, AIChE annual meeting, USA (2006).
16. I.G. Economou, A.N. Rissanou, L.D. Peristeras, “Molecular Simulation of Polymer Blends”, 22hd European Symposium on Applied Thermodynamics, Helsingor, Denmark (2006).
17. I.G. Economou, A.N. Rissanou, L.D. Peristeras and D.N. Theodorou, “Structure and Thermodynamic Properties of Linear - Tri-Arm Polyolefin Blends Based on Novel Atomistic Monte Carlo Simulation Schemes”, AIChE Annual Meeting, Session No 202, San Francisco, California, USA (2006).
18. L.D. Peristeras, I.G. Economou and D.N. Theodorou, "Elementary Moves in Monte Carlo Simulation of Linear and Branched Polyolefins", 19th European Seminar on Applied Thermodynamics, Santorini, Greece (2002).
19. L.D. Peristeras, M.K. Koukou, N. Papayannakos, N.C Markatos, "Design of a Full Scale Adiabatic Water Gas Shift Membrane Reactor", 1st European Congress on Chemical Engineering, ECCE1, Florence (1997).

## Student Advisement As Researcher At Demokritos

**Diploma Thesis students**

1. Leonidas Konstadopoulos (Academic advisor Prof. D.N. Theodorou, “A Monte Carlo computational study of conformational properties of polyethylene melts under elongational flow”, Department of Chemical Engineers, NTUA, 2021)

**Ph.D. students**

1. Giannis Diamataris (Advisory Committee, Academic advisor Asst. Prof. G.C. Boulougouris, Department of Molecular Biology & Genetics, Democritus University of Thrace, 2019-current)
2. Nastasia Lesgidou (Advisory Committee, Academic advisor Assoc. Prof. N.M. Glykos, Department of Molecular Biology & Genetics, Democritus University of Thrace, 2019-current)

## Reviewer

*Physical Chemistry Chemical Physics*, *European Polymer Journal*, *Chemical Engineering Science*, *Clays and Clay Minerals, Soft Matter, Polymers, Fuels*

## Selected Molecular Modeling Software

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| Amorphous Builder | A tool for creating initial configuration for molecular simulations. Developed in Computational Materials Science and Engineering Group (COMSE), integrated in Scienomics MAPS®, royalties program: 63154700, 15/3/2006 |
| Scienomics MAPS® | “Chameleon” a general Monte Carlo software for polymers, “Mesoscale Builder” a tool for creating coarse grain/mesoscale configuration of various morphologies, interface to LAMMPS, interface to MCCS-TOWHEE, simulation post process analysis, free/accessible volume analysis tool, molecular surface visualization tool |
| LAMMPS | Contribution of various interaction potentials, bug fixes |
| MCCCS-TOWHEE | Contribution for domain constrains used in insertion moves, bug fixes |
| PYSIMPP | Post-process functionality and utilities for molecular simulations |

## Selected Computer Skills

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| Management: | Clusters |
| Operating Systems: | Linux/Unix, MS-Windows |
| Programming: | C/C++, Java, Fortran, Python, Javascipt, bash, tcl, perl, etc. |
| Parallel Computing: | MPI, Open-MP, CUDA |