CURRICULUM VITAE: Dr. Loukas D. Peristeras
Chemical engineer, PhD

CURRENT

Special Research Scientist, Molecular Thermodynamics and Modelling of Materials Laboratory (MTMML), Institute of Nanoscience and Nanotechnology, NCSR "Demokritos"

CONTACT

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SCIENTIFIC RESUME

Prediction of macroscopic properties of materials with complex chemical constitution, molecular architecture and geometry using computations methods of molecular and thermodynamic modeling. Device algorithms and methods for the creation of initial configuration and the thermodynamic equilibration of complex molecular systems in various environments. Develop computation and end-user tools for promote and facilitate the application of these methods in industrial research and development activities.

GENERAL

Year of Birth:	1970
Nationality:	Hellenic
Gender:	Male
Military Obligations:	Fulfilled (1996-1998)

EDUCATION

2000-2003:	**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
1998-2000:	**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"
1989-1996:	**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

2014-curent:	**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

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 CO_2 (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 CO_2 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

SELECTED DEVELOPED SOFTWARE

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

SELECTED COMPUTER SKILLS

Administration:	Workstations, servers, clusters
Operating Systems:	Linux/Unix, MS-Windows
Programming:	C/C++, Java, Fortran, Python, Javascipt
Libraries API:	OpenGL, Qt, pthreads, Boost, CGAL, RDKit, OpenBabel
Parallel Computing:	MPI, Open-MP, CUDA
Modelling Software:	Accelrys Cerius[2], Scienomics MAPS®, Wolfram Mathematica, LAMMPS, GROMACS, NAMD, MCCCS TOWHEE, Amber

PUBLICATIONS LIST

1. M. Vasileiadis, **L. D. Peristeras**, K. D. Papavasileiou and I. G. Economou, Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization, *Energy & Fuels*, 2017, **31**, 6004–6018.
2. P. G. Takis, K. D. Papavasileiou, **L. D. Peristeras**, G. C. Boulougouris, V. S. Melissas and A. N. Troganis, Unscrambling micro-solvation of –COOH and –NH groups in neat dimethyl sulfoxide: insights from ^{1}H-NMR spectroscopy and computational studies, *Phys. Chem. Chem. Phys.*, 2017, **19**, 13710–13722.
3. L. F. Zubeir, M. A. A. Rocha, N. Vergadou, W. M. A. Weggemans, **L. D. Peristeras**, P. S. Schulz, I. G. Economou and M. C. Kroon, Thermophysical properties of imidazolium tricyanomethanide ionic liquids: experiments and molecular simulation, *Phys. Chem. Chem. Phys.*, 2016, **18**, 23121–23138.
4. R. T. J. Porter, H. Mahgerefteh, S. Brown, S. Martynov, A. Collard, R. M. Woolley, M. Fairweather, S. A. E. G. Falle, C. J. Wareing, I. K. Nikolaidis, G. C. Boulougouris, **L. D. Peristeras**, D. M. Tsangaris, I. G. Economou, C. Salvador, K. Zanganeh, A. Wigston, J. N. Najafali, A. Shafeen, A. Beigzadeh, R. Farret, P. Gombert, J. Hebrard, C. Proust, A. Ceroni, Y. Flauw, Y. Zhang, S. Chen, J. Yu, R. H. Talemi, J. Bensabat, J. L. Wolf, D. Rebscher, A. Niemi, B. Jung, N. M. Dowell, N. Shah, C. Kolster, E. Mechleri and S. Krevor, Techno-economic assessment of CO2 quality effect on its storage and transport: CO2QUEST: An overview of aims, objectives and main findings, *International Journal of Greenhouse Gas Control*, 2016, **54**, 662–681.

5. K. D. Papavasileiou, Z. A. Makrodimitri, **L. D. Peristeras**, J. Chen, G. P. van der Laan, I. Rudra, A. Kalantar and I. G. Economou, Molecular Simulation of *n* -Octacosane–Water Mixture in Titania Nanopores at Elevated Temperature and Pressure, *The Journal of Physical Chemistry C*, 2016, **120**, 24743–24753.
6. K. Nikolaidis, I. G. Economou, G. C. Boulougouris and **L. D. Peristeras**, Calculation of the phase envelope of multicomponent mixtures with the bead spring method, *AIChE Journal*, 2016, **62**, 868–879.
7. K. Nikolaidis, G. C. Boulougouris, **L. D. Peristeras** and I. G. Economou, Equation-of-State Modeling of Solid–Liquid–Gas Equilibrium of CO_2 Binary Mixtures, *Industrial & Engineering Chemistry Research*, 2016, **55**, 6213–6226.
8. S. Brown, **L. D. Peristeras**, S. Martynov, R. T. J. Porter, H. Mahgerefteh, I. K. Nikolaidis, G. C. Boulougouris, D. M. Tsangaris and I. G. Economou, Thermodynamic interpolation for the simulation of two-phase flow of non-ideal mixtures, *Computers & Chemical Engineering*, , DOI:10.1016/j.compchemeng.2016.09.005.
9. H. Tzoupis, G. Leonis, A. Avramopoulos, H. Reis, Ż. Czyżnikowska, S. Zerva, N. Vergadou, **L. D. Peristeras**, K. D. Papavasileiou, M. N. Alexis, T. Mavromoustakos and M. G. Papadopoulos, 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.
10. P. G. Takis, K. D. Papavasileiou**, L. D. Peristeras**, V. S. Melissas and A. N. Troganis, Probing micro-solvation in "numbers": the case of neutral dipeptides in water, *Physical Chemistry Chemical Physics*, 2013, **15**, 7354.
11. G. P. Lithoxoos, **L. D. Peristeras**, G. C. Boulougouris and I. G. Economou, Monte Carlo simulation of carbon monoxide, carbon dioxide and methane adsorption on activated carbon, *Molecular Physics*, 2012, **110**, 1153–1160.
12. G. P. Lithoxoos, A. Labropoulos, **L. D. Peristeras**, N. Kanellopoulos, J. Samios and I. G. Economou, 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**, 510–523.
13. G. C. Boulougouris**, L. D. Peristeras**, I. G. Economou and D. N. Theodorou, Predicting fluid phase equilibrium via histogram reweighting with Gibbs ensemble Monte Carlo simulations, *The Journal of Supercritical Fluids*, 2010, **55**, 503–509.
14. 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, *Polymer*, 2007, **48**, 3883–3892.
15. J. Ramos, **L. D. Peristeras** and D. N. Theodorou, Monte Carlo simulation of short chain branched polyolefins in the molten state, *Macromolecules*, 2007, **40**, 9640–9650.
16. **L. D. Peristeras**, A. N. Rissanou, I. G. Economou and D. N. Theodorou, 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**, 2904–2914.
17. **L. D. Peristeras**, I. G. Economou and D. N. Theodorou, Structure and Volumetric Properties of Linear and Triarm Star Polyethylenes from Atomistic Monte Carlo Simulation Using New Internal Rearrangement Moves, *Macromolecules*, 2005, **38**, 386–397.

CONFERENCES

1. 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)

2. 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)
3. 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)
4. **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)
5. I.G. Economou and **L.D. Peristeras**, "Calculation of Variable Architecture Polyolefin Miscibility from the Lattice Fluid Theory", 3rd Greek Chemical Engineering Conference, Athens, Greece (2001)
6. **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)

LANGUAGES

Greek, English

RECOMMENDATIONS

Upon request