

CURRICULUM VITAE

Personal Information

Name/Surname: George Papamokos

Current affiliation: Research Associate

IACM-FORTH

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Home Address: 30, Ioanninon Street

45221 Ioannina

Greece

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Military Service: Fulfilled

Marital Status: Married with two children.

Education

Ph.D. Computational Chemistry 2004, Department of Chemistry, Sector of Physical and Theoretical Chemistry University of Ioannina (excellent)

M.Sc. courses were completed successfully in 1998 with top marks. My research results were transferred to the PhD studentship.

B.Sc. in Chemistry, 1996, Department of Chemistry, University of Ioannina (Very Good)

Positions

➤ 15/01/2024 – 30/06/2024 Research Associate, School of Engineering and Applied Sciences, Harvard University, USA

➤ 09/02/2023-3/12/2023 Research Associate Department of Chemistry University of Ioannina

➤ 2021-2022 Lecturer (P. O. 407/80) Department of Chemistry, University of Ioannina

➤ 2021 Invited Researcher - Cyprus Institute (Computation-based Science and Technology Research Center (CaSToRC) (Inviting Researcher: Prof. V. Harmandaris)

➤ 2020-2021 Research Associate Laboratory of Biological Chemistry, Department of Medicine, University of Ioannina (Head Prof. A. Politou)

➤ 01/01/2020-20/01/2023 Research Associate Laboratory of Soft Matter, Dept. of Physics, University of Ioannina (Head Prof. G. Floudas)

➤ 16/09/2019-29/02/2020 Lecturer (P. O. 407/80) Department of Chemistry, University of Ioannina

- 01/10/2018-18/01-2019 University Scholar, Department of Chemistry, University of Ioannina
- 16/11/2016-12/02/2017 Greek Ministry of Education Experiencing Academic Teaching/Young Scientists: Department of Physics, University of Ioannina. Course: Biophysics
- 26/02/2015-30/09/2015 Research Associate Laboratory of Soft Matter, Dept. of Physics, University of Ioannina (Head Prof. G. Floudas)
- 2012-2014: Research Associate - International School for Advanced Studies (SISSA) – (Head Prof. C. Michelletti), Trieste, Italy and Guest of the German Research School for Simulation Sciences, Laboratory of Computational Biophysics, GmbH Jülich, Germany, Associated Research Scientist at the Institute for Advanced Simulations (IAS) Computational Biomedicine (IAS-5 / INM-9). Research in collaboration with Illy café. (Head Prof. P. Carloni)
- 2010 July-Dec.: Research Scientist, École Polytechnique Fédérale de Lausanne (EPFL), School of Engineering, EPFL-STI-IMX-LMMM (Head Prof. E. Kaxiras)
- 2007-2010: Visiting Lecturer, University of Western Macedonia, Greece
- Oct. 2006-Jan. 2007: Visitor Research Scholar, Department of Physics, Harvard University, USA
- Apr. 2005-Apr. 2006: Postdoctoral Researcher, Biomedical Research Institute, FORTH-BRI & Laboratory of Biological Chemistry, Medical School, University of Ioannina, Greece (Head Prof. A. Politou)
- Feb. 2004-Aug. 2008: Academic Projects Coordinator, Technological Educational Institute of Epirus
- 2002-2008 & 2010-2012: Laboratory Teaching staff and visiting Assistant Professor, Technological Educational Institute of Epirus

Funding Summary and Honors

2023 ELIDEK – In-Cell NMR (Head: Prof. I. Gerothanassis)

2021-2022 ELIDEK-POLYCONF: Polymer dynamics under 2D confinement (Head: Prof. G. Floudas)

2020–2021 "ELIXIR-GR: ELIXIR-GR: Managing and Analyzing Life Sciences Data." (Head Prof. A. Politou)

<https://elixir-europe.org/about-us/who-we-are/nodes/greece>

2020-2021 – Effect of confinement on the structure and the dynamics of soft matter Ministry of Development and Investments (Head: Prof. G. Floudas)

2018-2019: University Scholar, Department of Chemistry, University of Ioannina

2016: Greek Ministry of Education Experiencing Academic Teaching/Young Scientists: Department of Physics, University of Ioannina. Course: Biophysics

2015: Greek Ministry of Education (ESPA Thalys program)

2012: International Research Scholarship SISSA and E. Illy foundation

2012: Greek Ministry of Education (ESPA Heraclitus II program) *declined*

Oct 2006-Jan 2007: Visitor Research Scholar, Lyman Laboratory, Department of Physics, Harvard University

Apr. 2005 Apr. 2006: Ministry of Education (EPEAEK Pythagoras II program)

Jan. 2000 -Dec. 2000: Interreg II, Greece-Italy, Graduate Scholarship, transferred to Chemistry Department - University of Calabria, Italy (two months visit Oct-Noe 2000)

1993-1994: ERASMUS-ECTS Scholarship, transferred to the Chemistry Department "at Trinity College of Dublin" Ireland

1991: **Achieved 5th best score, Greek Entrance Examinations, Chemistry Department, University of Ioannina**

Teaching Activities

Master and Ph.D.

- Winter Semester 2019-2021: Master program Molecular Cell Biology and Biotechnology Medical School, University of Ioannina
- Winter Semester 2012-2013: German Research School for Simulation Sciences, Master's program in Simulation Sciences (Instructor)
- Winter Semester-2010: Training of Master and Ph.D. students for High-Performance Computing and MD simulations EFPL-STI-IMX-LMMM

Undergraduate

2023-2024 Co-supervisor of an undergraduate student in research activities relative to epigenetics (Student: **Natalie Martin** Harvard College, Class of 2024 A.B. Candidate in Chemistry & Physics)

- 2019-2020 (Winter Semester) Adjunct Professor, Department of Chemistry, University of Ioannina Course: "Informatics for Chemists"
- 2018-2019 (Winter Semester) Adjunct Professor, Department of Chemistry, University of Ioannina Course: "Informatics for Chemists"
- 2016-2017 (Winter Semester) Lecturer, Department of Physics, University of Ioannina Course: "Biophysics"
- 2015-2016: Invited Lecturer, (invitation sent by Assoc. Prof. M. Fragou-Lazaridis) School of Medicine, University of Ioannina, Course: "Biotechnology – Molecular Diseases"
- 2007-2010: Visiting Lecturer, Department of Informatics and Telecommunications Engineering, University of Western Macedonia, Courses: "Databases", Multimedia Technologies"

- 2009-2010: Invited Lecturer, (invitation sent by Ass. Prof. A. Politou) Department of Biological Applications and Technologies, University of Ioannina, Course: "Structural Biology"
- 2002-2008 and 2010-2012: Visiting Laboratory Assistant and Assistant Professor, Technological Institute of Epirus, Department of Informatics, Department of Nursing and School of Agricultural Technology, Courses: "Nanotechnology", "Bioinformatics", "Networks"
- 2002-2003: Assistant Teaching Staff, Department of Biological Applications and Technologies, University of Ioannina
- 1998-2000: Assistant Teaching Staff, Department of Chemistry, University of Ioannina, Course: "Introduction to Computer Science and Programming"
- 1998-1999: Assistant Teaching Staff, Department of Chemistry, University of Ioannina, Course "Laboratory of Physical Chemistry I"
- 1997-2000: Assistant Teaching Staff, Department of Chemistry, University of Ioannina, Course: "Laboratory of Physical Chemistry II", and Course: "Quantum Chemistry"

Supervision of undergraduate and graduate students in Greek Universities:

Supervisor or co-supervisor of more than 6 Bachelor Theses. One of them was published in "Computers in Biology and Medicine" and two of them in "Ang. Chem. Int. Ed.", "ACS Appl. Mater. Interfaces" journals.

Other

- Organizer and Instructor of Summer Seminars 2022 on Computational Biochemical Tools and Methods for undergraduate and postgraduate students under the auspices of the Institute of Biosciences – University Research Center of Ioannina (I.B.S.-URC-Ioannina)

I have organized an educational seminar series on computational biochemistry for undergraduate and postgraduate students at the University of Ioannina, emphasizing molecular docking, the prediction of protein structure based on artificial intelligence, and computational toxicology.

https://urci.unit.uoi.gr/ibs/files/Summer%20seminars%20-IBS_URC_Ioannina_v3.pdf
<https://urci.unit.uoi.gr/ibs/en/index.html>

Track Record

A. Peer-Reviewed Journal Publications

- A43.** T. Venianakis, T. Goričanb, **G. Papamokos**, S. Golič Grdadolnikb, Michael Siskos, and Ioannis P. Gerothanassis* Are the pKa values of free fatty acids in aqueous solution abnormally high? A combined NMR, DFT, and MD study. *In preparation*
- A42.** S. Pathreker, C. A. Snyder, **G. Papamokos**, and R. J. Composto The Effect of Boron Nitride Flakes on Sodium Ion Transport in PEO Electrolytes *Accepted*
- A41.** C-H Tu, E. Fastow, R. J. Chethalen, **G. Papamokos**, B. Coughlin, and K. I. Winey, Coupling, and Decoupling between Stickers and Backbones in Associating Polymers with Terminally Functionalized Side Chains *In revision*
- A40.** Chalkidou, P. Venianakis, T. **Papamokos**, G. Siskos, M. and Gerothanassis, I. P. Can we predict a "magic" number of catalytically important water molecules in H/D exchange in aromatic systems? A combined NMR and DFT study *Submitted*
- A39.** N. Patsalidis, **G. Papamokos**, G. Floudas, and V. Harmandaris Temperature Dependence of the Dynamics and Interfacial Width in Nanoconfined Polymers via Atomistic Simulations *J. Chem. Phys.* 160, 104904 (2024)
- A38.** Pathreker, S. Snyder, C. A. **Papamokos**, G. Composto, R. J. Hexagonal Boron Nitride Modulates Crystallinity and Charge Mobility in PEO–NaNO₃ Electrolytes. *J. Phys. Chem. C*, **2024**, 128, 1, 38–49.
- A37.** T. Venianakis, A. Primikyri, T. Opatz, S. Petry, **G. Papamokos**,* and I. P. Gerothanassis* NMR and Docking Calculations Reveal Novel Atomistic Selectivity of a Synthetic High-Affinity Free Fatty Acid vs. Free Fatty Acids in Sudlow's Drug Binding Sites in Human Serum Albumin *Molecules*, **2023**, 28, 7991.
- A36.** Venianakis, T.; Siskos, M.G.; **Papamokos**, G.*; Gerothanassis, I.P. Structural Studies of Monounsaturated and ω -3 Polyunsaturated Free Fatty Acids in Solution with the Combined Use of NMR and DFT calculations -Comparison with the Liquid State. *Molecules*, 28 6144 **2023**
- A35.** N. Patsalidis, **G. Papamokos**, G. Floudas, and V. Harmandaris Structure and dynamics of Polybutadiene melt confined into Alumina substrates *Macromolecules* **2023** 56 (16), 6552-6564.
- A34.** **G. Papamokos*** E. Kaxiras* How to evict HP1 from H3: Using a double salt bridge *Biophysical Chemistry* 123, 27 α , **2023**.
- A33.** Eleni Alexandri, Themistoklis Venianakis, Alexandra Primikyri, **Georgios Papamokos*** and Ioannis P. Gerothanassis* Molecular Basis for the Selectivity of EPA and DHA in Human Serum Albumin with the Combined Use of NMR and Docking Calculations. *Molecules* **2023**, 28, 3724.
- A32.** T. Venianakis, M. Siskos, **G. Papamokos*** and I. P. Gerothanassis* NMR and DFT studies of unsaturated free fatty acids in the liquid state reveal a unique atomic-level structural model of DHA *J. Mol. Liquids* **2023**, 376, 121459.
- A31.** A. Primikyri, M. Sakka, V. Kontogianni, G. Papamokos and I. P. Gerothanassis Structural basis of artemisinin binding sites on serum albumin and conformational characterization with IN PHARMA NMR and docking calculations *Molecules* 27, **2022**, 5912.
- A30.** N. Patsalidis, **G. Papamokos***, G. Floudas, and V. Harmandaris* Understanding the Interaction between Polybutadiene and Alumina via DFT Calculations and Machine-learned Atomistic Simulations *ACS Journal of Physical Chemistry* **2022**

- A29.** E. Alexandri, A. Primikyri, **G. Papamokos** and I. P. Gerothanassis. NMR and computational studies reveal atomic-level molecular recognition of unsaturated fatty acids with non-labeled albumin. *FEBS Journal* **2022** 289 (18), 5617-5636
- A28.** M. Spyridakou, C. Gardiner, G. Papamokos, H. Frey* and G. Floudas. Dynamics of Poly(cyclohexene carbonate) as a Function of Molar Mass. *ACS Applied Polymer Materials* **2022**
- A27.** A. Ananiadou, **G. Papamokos**, M. Steinhart and G. Floudas. Effect of confinement on the dynamics of 1-propanol and other monohydroxy alcohols. *J. Chem. Phys.* **155**, **2021**, 184504.
- A26.** T. Venianakis, A. Primikyri, E. Alexandri, **G. Papamokos*** and I. P. Gerothanassis* Molecular models of three ω -3 fatty acids based on NMR and DFT calculations of ^1H NMR chemical shifts" *Journal of Molecular Liquids* **342**, **2021**, 117460.
- A25.** **G. V. Papamokos*** G. Tziatzos, D. G. Papageorgiou, S. D. Georgatos, E. V. Kaxiras, A. Politou.* Progressive Phosphorylation Dictates the Self-Association of a Variably Modified Histone H3 Peptide. *Frontiers in Molecular Biosciences* **2021**, **8**, Article no 698182
- A24.** A. Pipertzis, **G. Papamokos**, S. Oskar, U. Scherf*, G. Floudas.* Ionic Conductivity in Polyfluorene-based Diblock Copolymers comprising Nano-domains of a Polymerized Ionic Liquid and a Solid Polymer Electrolyte Doped with LiTFSI. *Macromolecules* **2021**, **54** (9), 4257-4268.
- A23.** A. Theodoridis, **G. Papamokos**, M. P. Wiesenfeldt, M. Wollenburg, K. Müllen, F. Glorius, G. Floudas* Polarity Matters: Dielectric Relaxation in all-*cis*-Multifluorinated Cycloalkanes. *J. Phys. Chem. B* **2021**, **125** (14), 3700-3709
- A22.** A. Ananiadou, **G. Papamokos**, M. Steinhart, G. Floudas. Nanometer Confinement Induces Nematic Order in 1-Dodecanol. *J. Phys. Chem. B* **2020**, **124**, 10850-10857.
- A21.** A. Pipertzis, **G. V. Papamokos**, M. Mühlinghaus, M. Mezger, U. Scherf, * G. Floudas.* What Determines the Glass Temperature and Dc-Conductivity in Imidazolium Polymerized Ionic Liquids with a Polythiophene Backbone? *Macromolecules* **2020**, **53**, **9**, 3535–3550
- A20.** **Papamokos G.*** Dimitriadis T., Bikiaris D. N., Papageorgiou G. Z., Floudas G*. Chain Conformation, Molecular Dynamics, and Thermal Properties of Poly(n-methylene 2,5-furanoates) as a Function of Methylene Unit Sequence Length *Macromolecules*, **2019**, **52**, 6533-6546
- A19.** Selevou A., **Papamokos G.**, Yildirim T., Duran H., Steinhart M., Floudas G. Eutectic Liquid Crystal Mixture E7 in Nanoporous Alumina. Effects of Confinement on the Thermal and Concentration Fluctuations. *RSC Adv.* **2019**, **9** (65), 37846-37857.
- A18.** **G. V. Papamokos*** The nature of biological material and the irreproducibility problem in biomedical research. *EMBO J.* **2019** e101011 (commentary - reviewed by the board of directors)
- A17.** **G. V. Papamokos** J. Wudarczyk, R. Graf, D. Schollmeyer, M. Baumgarten, G. Floudas, K. Müllen. Dipolar relaxation in functionalized poly-*p*-phenylenes bearing

ultra-strong dipoles perpendicular to the backbone. *Macromolecules*, **2018** 51 3330–3339.

A16. A. Pipertzis, A. Hess, P. Weis, **G. Papamokos**, K. Koynov... G. Floudas. Multiple segmental processes in polymers with cis and trans stereoregular configurations. *ACS Macro Letters* **2018**, 7, 11-15.

A15. A. Selevou, **G. Papamokos**, M. Steinhart, and G. Floudas 8OCB and 8CB Liquid Crystals Confined in Nanoporous Alumina. Effect of Confinement on the Structure and Dynamics. *J. Phys. Chem. B*, **2017**, 121 7382–7394

A14. S. Alexandris, A. Franczyk, **G. V. Papamokos**, B. Marciniak, K. Matyjaszewski, K. Koynov, G. Floudas. Dynamic Heterogeneities in Random Copolymers of two Polymethacrylates with Polyhedral Oligomeric Silsesquioxane Moieties (POSS) *Macromolecules*, **2017**, 50, 4043–4053.

A13. J. Wudarczyk, **G. V. Papamokos**, T. Marszalek, T. Nevolianis, D. Schollmeyer, F. Hinkel, W. Pisula, G. Floudas, M. Baumgarten and K. Müllen. Dicyanobenzothiadiazole Derivatives Possessing Switchable Dielectric Permittivities. *ACS Appl. Mater. Interfaces*, **2017**, 9, 20527–20535.

A12. **G. V. Papamokos** and I. Silins. Combining QSAR Modeling and Text-Mining Techniques to Link Chemical Structures and Carcinogenic Modes of Action *Frontiers in Pharmacology* **2016**, 7, 284. (open)

A11. J. Wudarczyk, **G. V. Papamokos**, V. Margaritis, D. Schollmeyer, M. Baumgarten, G. Floudas and K. Müllen. Hexasubstituted Benzenes bearing Ultrastrong Dipole Moments. (Communication) *Ang. Chem. Int. Ed.* **2016**, 55, 3220-3223. [Included in top research 2016 of the ACS](http://yearinreview.cenmag.org/top-research-of-2016/) <http://yearinreview.cenmag.org/top-research-of-2016/>

A10. Alexandris S., Franczyk A., **Papamokos G. V.**, Marciniak B., Matyjaszewski K., Koynov K., Mezger M., Floudas G. Polymethacrylates with Polyhedral Oligomeric Silsesquioxane Moieties (POSS): The Influence of Spacer Length on Packing, Thermodynamics, and Dynamics. *Macromolecules* **2015**, 48, 3376-3385.

A9. N. D. Amelio, **G. V. Papamokos**, J. Dreyer, L. Navarini, P. Carloni. ¹H NMR studies of hetero-association of caffeine with di-O-caffeoylquinic acid isomers in aqueous solution. *Food Biophysics*, **2015**)

A8. Vlachopoulos A., Soupsana E., Politou A., **Papamokos G. V.*** Potamos Mass Spectrometry Calculator: Computer-Aided Mass Spectrometry to the Post-Translational Modifications of Proteins. A Focus on Histones. *Computers in Biology and Medicine*, **2014**, 55, 36-41 <http://potamos.seas.harvard.edu> <http://imbb.forth.gr/potamos> <https://potamos.med.uoi.gr/>

A7. Stanyon H., Cong X., Chen Y., Shahidullah N., Rossetti G., Dreyer J., **Papamokos G.**, Carloni P., Viles J. Developing predictive rules for coordination geometry from visible circular dichroism of Copper(II) and Nickel(II) ions in histidine and amide main-chain complexes. *FEBS Journal*, **2014**, 281, 3945-3954

A6. G. Papamokos, J. Dreyer, L. Navarini, P. Carloni. Trapping acrylamide by a Michael addition: A computational study of the reaction between acrylamide and niacin. *Int. J. Quant. Chem.* **2014**, 114, 553-559)

A5. Papamokos G. V., G. Tziatzos, D. G. Papageorgiou, S. D. Georgatos, A. S. Politou, E. Kaxiras. Structural role of RKS motifs in chromatin interactions: an MD study of HP1 bound to a variably modified histone tail. *Biophys. J.* **2012**, 102, 1926-1933.

A4. Papamokos G. V., I. G. Tsoulos, I. N. Demetropoulos, E. Glavas. Location of amide I mode of vibration in computed data utilizing constructed neural networks. *Expert systems with applications*. **2009**, 36, 12210-12213.)

A3. Papamokos, G.V., and Demetropoulos, I. N.; Biomolecular Springs: Low-Frequency Collective Helical Vibrations of Ace-Gly_n-Nme (n=3-8). A DFT Study Employing the PW91_{xc} Functional. *J. Phys. Chem. A* **2004**, 108, 8160-8169.

A2. Papamokos, G.V., and Demetropoulos, I. N.; Vibrational Frequencies of Amides and Amide Dimers: The assessment of PW91_{xc} Functional. *J. Phys. Chem. A* **2004**, 108, 7291-7300.

A1. Papamokos, G.V., and Demetropoulos, I. N.; Multitask Molecular Springs: Collective Helical Vibrations of R₂S_n (R = H, C₆H₅, C₂H₃, CCl₃). A Quantum Mechanical Study *J. Phys. Chem. A* **2002**, 106(9), 1661-1669.

Ac. Cover art pages:

https://biophysicalsociety.files.wordpress.com/2012/04/bpj102_8.jpg

<https://pubs.acs.org/toc/jpcck/126/39>

Am. Media

<http://biophysicalsociety.wordpress.com/2012/04/16/histone-tails-on-the-biophysj-cover/>

http://www.fondazionernestoilly.org/en_US/lattivita/scientific-projects/ricerca-sulla-tossicologia-computazionale/

<https://www.chemistryworld.com/news/a-small-molecules-big-moment/9432.article>

B. Peer-Reviewed International Conference Publications, Workshops

B27. Decoupled Main-Chain and Sticker Dynamics in Associating Comb Polymers CH Tu, E Fastow, R Chethalen, **G Papamokos**, B Coughlin, K Winey **Bulletin of the American Physical Society** **2024**

B26. Unravelling the mechanism of HP1 eviction from methylated Histone H3: A DFT study suggests a complex salt bridge as the spurring interaction **G Papamokos**, E Kaxiras **Bulletin of the American Physical Society** **2024**

B25. Hexagonal Boron Nitride Modulates Crystallinity and Charge Mobility in PEO–NaNO₃ Electrolytes C Snyder, S Pathreker, **G Papamokos**, R Composto **Bulletin of the**

American Physical Society 2024

B24. N. Patsalidis, **G. Papamokos**, G. Floudas, V. Harmandaris Structure and Dynamics of Polymer Chains in Polymer/Alumina Interfaces via Machine-Learnt Atomistic Simulations 5th International Conference on Structural Nano Composites NANOSTRUC 2023 Novel Materials for Future 24-26 May 2023 Nicosia, Cyprus

B23. N. Patsalidis, **G. Papamokos**, G. Floudas, and V. Harmandaris. Properties of Polybutadiene Melts Adsorbed in Alumina via a hierarchical multi-stage simulation methodology - Stimulate European Joint Doctorates Conference on simulations in Multiscale Physical and Biological Systems 22-26 November 2021 Almyra Hotel, Pafos, Cyprus.

B22. Elixir -SAC 2021: ELIXIR-GR, Ioannina node - Potamos Mass Spectrometry Calculator **G. Papamokos**, A. Vlachopoulos, A. Politou

B21. A. Pipertzis, **G. Papamokos**, M. Muhlinghaus, O. Sachnik, M. Mezger, U. Scherf, G. Floudas Mechanism of Ion Transport in Imidazolium Polymerized Ionic Liquids (PILs) Bearing a Polythiophene Backbone and in Dual Ionic Conductors of Polyfluorene Block Copolymers Doped with LiTFSI. APS March Meeting 2021 *Bulletin of the American Physical Society*

B20. **G. Papamokos**, I. Silins. Linking QSAR and mode of action data to improve the prediction of carcinogens. HBIO 216 19-21 November 2016, Thessaloniki, Greece (oral)

B19. **G. Papamokos**, G. Tziatzios, D. Papageorgiou, S. Georgatos, E. Kaxiras, A. S. Politou. Computational epigenetics of histone H3: MD studies of combinatorial modification patterns on the H3 tail. 67th Panhellenic Conference-Hellenic Society of Biochemistry and Molecular Biology 25-27 November 2016, Ioannina, Greece (oral)

B18. **G. Papamokos**, I. Silins. Linking QSAR and mode of action data to improve the prediction of carcinogens. 67th Panhellenic Conference-Hellenic Society of Biochemistry and Molecular Biology 25-27 November 2016, Ioannina, Greece (poster)

B17. A. Vlachopoulos, E. Soupsana, A. S. Politou. **G. Papamokos**. POTAMOS mass spectrometry calculator: Computer-aided mass spectrometry to the post-translational modifications of histones 67th Panhellenic Conference Hellenic Society of Biochemistry and Molecular Biology 25-27 November 2016, Ioannina, Greece (poster)

B16. T. Nevolianis, J. Wudarczyk, **G. Papamokos** K. Müllen & G. Floudas. Polymers of hexasubstituted benzenes bearing ultrastrong dipole moments. XXXII Panhellenic Conference on Solid State Physics and Materials Science. 18-21 September 2016, Ioannina, Greece (poster)

B15. V. Margaritis, J. Wudarczyk, K. Muellen, **G. Papamokos**, G. Floudas. Designing Molecules for Organic Photovoltaics: The case of Hexasubstituted Benzenes carrying Ultrastrong Dipole Moments. XXXI Panhellenic Conference on Solid State Physics and Materials Science. Thessaloniki. September 2015. (poster)

- B14.** S. Alexandris, A. Franczyk, **G. Papamokos**, B. Marciniak, K. Matyjaszewski, K. Koynov, M. Mezger, and G. Floudas "Polymethacrylates with Polyhedral Oligomeric Silsesquioxane Moieties (POSS): The Influence of Spacer Length on Packing, Thermodynamics and Dynamics" XXXI Panhellenic Conference on Solid State Physics and Materials Science Thessaloniki, 20-23 September 2015. (poster)
- B13.** **G. Papamokos (invited speaker)**, V. Margaritis, J. Wudarczyk, K. Muellen, G. Floudas. Employing DFT methods for designing molecules with ultra-strong dipole moments. Workshop on «Mathematical and Computational Techniques for Molecular Systems» Institute of Applied and Computational Mathematics, FORTH, Heraklion ACMAC Center, University of Crete, Heraklion 16-18 September 2015 (oral)
- B12.** **G. V. Papamokos** V. Margaritis, J. Wudarczyk, K. Muellen, G. Floudas. Designing Molecules for Organic Photovoltaics: Hexasubstituted Benzenes with Ultrastrong Dipole Moments Workshop on "Self-Assembly in Soft Matter" Conference Center, University of Patra Tuesday and Wednesday, Sept. 1st & 2nd, 2015 (oral)
- B11.** **G. V. Papamokos**, G. Tziatzos, A. Politou, D. Papageorgiou, S. Georgatos, E. Kaxiras. "Computational Epigenetics: Molecular dynamics simulations of the structure of HP1 bound to a variably modified histone tail." 55th Annual Meeting, Baltimore, Maryland, March 5-9, 2011. *Biophysical Journal* 100(3) pp. 228a. (poster)
- B10.** Y. Markaki, A. Christogianni, **G. Papamokos**, A. S. Politou, and S. D. Georgatos (2008). An Editable Modification Pattern that Marks and Configures Mitotic Chromatin. 33rd FEBS Congress - 11th IUBMB Conference, Athens, Greece. *FEBS JOURNAL* 2008, 275, 458. ([pdf](#)) (poster)
- B9.** Y. Markaki, A. Christogianni, **G. Papamokos** A.S. Politou, S.D. Georgatos (2006). A H3 modification pattern that marks and configures mitotic chromatin, 16th Meeting of Methods in Protein Structural Analysis, Lille, France. MPSA 2006 Abstract 12, p. 50 (poster)
- B8.** G. Tziatzos, **G. V. Papamokos**, D. Papageorgiou. Molecular Dynamics study of post-translational modifications in the H3-HP1 complex. 4th Conference of the Greek Society of Computational Biology and Bioinformatics 18-20 Dec. 2009, National Institute of Research, Athens, Greece. (oral; speaker: G. Tziatzios)
- B7.** **G. V. Papamokos**, G. Tziatzos, D. Papageorgiou, A. Politou and [E. Kaxiras](#). Computational Epigenetics: Molecular simulations of the structure of HP1 bound to a variably modified H3 tail: A binary switch or a modification cassette? 4th Conference of the Greek Society of Computational Biology and Bioinformatics 18-20 Dec. 2009, National Institute of Research, Athens, Greece. (oral)
- B6.** Y. Markaki, A. Christogianni, **G. Papamokos**, A. S. Politou and S. D. Georgatos (2007). Phosphorylation of Histone H3 Establishes an Editable Modification Pattern that Marks and Configures Mitotic Chromatin. 59th Meeting of the Hellenic Society for Biochemistry

and Molecular Biology, Athens, Greece (**3rd prize for oral presentation – speaker: Y. Markaki**)

B5. Y. Markaki, A. Christogianni, **G. Papamokos**, A.S. Politou, S.D. Georgatos (2006). Phosphorylation of histone H3 establishes an editable modification pattern that marks and configures mitotic chromatin, *58th Meeting of the Hellenic Society of Biochemistry and Molecular Biology, Patras, Greece. oral presentation – speaker: Y. Markaki*

B4. **G. V. Papamokos**, I. G. Tsoulos, I. N. Demetropoulos, E. Glavas. Structural Bioinformatics: An automated recognition algorithm of collective helical vibrations. 20th Pan-Hellenic Conference of Chemistry, Ioannina, September 2005, p. 90, oral presentation)

B3. **G. V. Papamokos**, I. N. Demetropoulos. Novel collective vibrations in molecular helices of biological interest. 19th Pan-Hellenic Conference of Chemistry, Heraklion, November 2002, (p. 648-651 poster).

B2. **G. V. Papamokos**, I. N. Demetropoulos. Molecular multifunctional springs: Collective helical vibrations of R_2S_n ($R=H, C_6H_5, C_2H_5, CCl_3$). 18th Pan-Hellenic Conference of Chemistry, Piraeus March 2001, (p. 389-392 oral presentation).

B1. **G. V. Papamokos**, I. N. Demetropoulos. Polysulfanes: A computational study of architectures comprising intramolecular parallel helices. 18th Pan-Hellenic Conference of Chemistry, Patra, December 1996, (p. 659-662 – oral presentation).

C. University of Ioannina Conferences

Published four posters and two oral presentations. For one of them, our team was awarded the **1st prize**.

C1. **G. V. Papamokos**, C. Dimakopoulos, N. Russo, I. N. Demetropoulos. Quantum investigation of the main stages of the protein folding: Structural transformation of the oligopeptide (Ala)₄ from an alpha-helical structure to a 3₁₀-helical structure.

12th Macedonian Conference of Nutrition and Dietetics

D2. **G. Papamokos**, I. Silins. Combining chemoinformatics methods (QSAR) and text mining techniques to link chemical structures and carcinogenic mode of action of toxic chemicals found in food and the environment. *12th Macedonian Conference of Nutrition and Dietetics, Thessaloniki, Greece, 11-13 May 2018 (oral)*

D1. **G. Papamokos**, J. Dreyer, L. Navarini, and P. Carloni. Inhibiting the action of toxic chemicals in food through dietetics. A computational study of the reaction between acrylamide and niacin *12th Macedonian Conference of Nutrition and Dietetics, Thessaloniki Greece 11-13 May 2018 (oral)*

Review Editor for

- Frontiers in Chemistry
Section: **Theoretical and Computational Chemistry**

Reviewer for the journals:

- Certified Reviewer of the American Chemical Society
- ACS Macromolecules
- ACS Journal of Proteome Research
- ChemPhysChem - Wiley
- PhysChemChemPhys - RSC
- Current Medicinal Chemistry
- Peer J (<https://peerj.com/life-environment/>)
- J. Mol Graphics and modeling

Spoken Languages

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