

## CURRICULUM VITAE

### Anastassia Rissanou

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#### EDUCATION

- **PhD** in Simulation studies on Polymeric and Colloidal Systems, Department of Physics, University of Crete, Heraklion Crete, Greece (2003).
- **M.Sc.** in Condensed Matter Physics, Department of Physics, University of Crete, Heraklion Crete, Greece (1998).
- **B.Sc.** degree in Physics, Department of Physics, University of Crete, Heraklion Crete, Greece (1996).

#### PROFESSIONAL EXPERIENCE AND APPOINTMENTS

- 11/2022 - present: Associate Researcher (Grade C), Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Greece.
- 01/2022 – 10/2022: Collaborating Researcher in The Cyprus Institute, Computation-based Science and Technology Research Center, Nicosia, Cyprus.
- 10/2017-12/2021 : Collaborating Researcher in the Institute of Applied and Computational Mathematics (IACM) - Foundation for Research and Technology Hellas (FORTH), Heraklion, Crete. Research Program: "THE GOODYEAR TIRE & RUBBER COMPANY".
- 05/2020 – 07/2021: Collaborating Researcher in Foundation for Research and Technology Hellas, Institute of Electronic Structure and Laser (EDBM 103).

- 03/2019 –03/2021: Collaborating Researcher in Aristotle University of Thessaloniki, Department of Chemical Engineering in the framework of ESPA 2014-2020 Operational Program Competiveness-Entrepreneurship-Innovation.
- 10/2015-11/2016: Collaborating Researcher: Crete Center for Quantum Complexity and Nanotechnology (CCQCN), Department of Physics, University of Crete, Heraklion, Crete.
- 04/2013-09/2013: Post-Doctoral Researcher: in University of Crete, Archimedes Center for Analysis, Modeling & Computation.
- 12/2011-07/2012: Post-Doctoral Researcher: Foundation for Research and Technology Hellas, «Graphene Center».
- 08/2007-09/2008: Post-Doctoral Researcher: Foundation for Research and Technology Hellas, Institute of Electronic Structure and Laser and Institute für Theoretische Physik II Heinrich-Heine-Universität Düsseldorf, Germany.
- 10/2003-07/2007: Post-Doctoral Researcher: NRCPS “Demokritos” - Institute of Physical Chemistry - Molecular Thermodynamics and Modelling of Materials Laboratory.
- 10/2005-12/2005: Visiting Researcher in Chemical Engineering Department of Princeton University, Princeton, New Jersey, USA.

### MAIN RESEARCH INTERESTS

- **Computational Modeling:** Multi-scale simulation techniques, atomistic and mesoscopic modeling. Molecular dynamics, Monte Carlo, Stochastic dynamics, Brownian dynamics. Development of new computer simulation methods. Machine Learning Techniques.
- **Soft Materials:** Simulation studies on static, conformational and dynamic properties of polymers and colloids with the use of various computational methods.
- **Biological Systems:** Simulation studies of short peptides; Proteins (mutations) ; RNA (Drug design problem).
- **Complex Materials:** Simulation studies of nanocomposites : Polymer-Graphene nanocomposites; Polymer-Silica nanocomposites; Peptide-Graphene nanocomposites.

### EXTERNAL FUNDING

- Molecular Simulations of Polymers for Tire Materials “THE GOODYEAR TIRE & RUBBER COMPANY”, Collaborating Researcher (10/2017-31/12/2021).
- Innovative nano-hyperparamagnetic ribonucleoprotein navigators for tailored treatment of breast cancer, ESPA 2014-2020 Operational Program Competiveness-Entrepreneurship-Innovation, Collaborating Researcher (06/03/2019-30/03/2021).

- Development of computer simulation models for nanosheets of graphite oxide and corresponding polymer nanocomposites, Operational Program Competiveness-Entrepreneurship-Innovation ESPA 2014-2020”, Collaborating Researcher (01/05/2020-31/07/2021).

### TEACHING EXPERIENCE

**2010-2013:** Assistant Professor (PD 407) in the Department of Mathematics and Applied Mathematics, University of Crete, Heraklion, Greece.

**2007-2011:** Visiting (hourly rated) professor: in the Hellenic Mediterranean University, Heraklion/Rethymno, Crete, Greece.

**2006-2007:** Visiting (hourly rated) professor in School of Pedagogical and Technological Education (ASPETE), Heraklion, Crete, Greece.

### PROFESSIONAL AFFILIATIONS & ACTIVITIES

#### Memberships:

- American Physical Society (APS)
- Hellenic Polymer Society
- European Colloid & Interface Society
- Hellenic Society for the Science and Technology of Condensed Matter

**Topic Editor in International Journal of Molecular Sciences Special Issue:** New Topic: Fibrous Proteins and Self-Assembling Peptides: From Structure and Assembly to Applications [Biomolecules, IJMS, Nanomaterials, Viruses]

#### **Reviewer in 20 International Scientific Journals**

### AWARDS AND DISTINCTIONS

#### ***Four Publications have distinguished for covers in the following International Journals***

- "Investigation of the properties of nanographene in polymer nanocomposites through molecular simulations: dynamics and anisotropic Brownian motion", A. N. Rissanou, P. Bacova, V. Harmandaris, ***Physical Chemistry Chemical Physics*** 21, 23843-23854 (2019).
- "All-atom Molecular Dynamics Simulations of Single Stranded RNA with an Ionizable Complexation", A. N. Rissanou, A. Ouranidis, K. Karatasos, ***Soft Matter***, 16, 6993-7005 (2020).
- "Self-assembly of Alanine-Isoleucine and Isoleucine-Isoleucine Dipeptides through Atomistic Simulations and Experiments", A. N. Rissanou, G. Simatos, P. Siachouli, V. Harmandaris, A. Mitraki, ***J. Phys. Chem. B***, 124, 33, 7102–7114 (2020).

- “Polybutadiene Copolymers via Atomistic and Systematic Coarse-Grained Simulations” A. Rissanou, A. Chazirakis, P. Polinska, C. Burkhart, M. Doxastakis, V. Harmandaris, *Macromolecules*, 55 (1), 224-240 (2022).

<b>2019 July Invited Talk</b>	Anastassia Rissanou, V. Harmandaris, A. Ouranidis, K. Karatasos “Structure and Self-Assembly of Biomolecules through Molecular Simulations”, 16 <sup>th</sup> International Conference on Nanosciences & Nanotechnologies (NN19), Thessaloniki, (July 02-05) 2019.
<b>2018 July Invited Talk</b>	Anastassia Rissanou, Vagelis Harmandaris “Nanographene Sheets as Fillers in Polymer Matrices: A Molecular Dynamics Study”, 15 <sup>th</sup> International Conference on Nanosciences & Nanotechnologies (NN18), Thessaloniki, Greece (July 03-06) 2018.
<b>1996 July:</b>	<b>3rd award</b> (after examination): 8th Summer School organized by the Physics Department of University of Crete.
<b>1995 July:</b>	<b>6th award</b> (after examination): 7th Summer School organized by the Physics Department of University of Crete.

## PUBLICATIONS

- **37** publications in highly ranked international journals.
- **31** publications in refereed conference proceedings.
- **2** publications in book chapters.
- Participation in more than **100** national and international conferences.  
About **70** presentations by Anastassia Rissanou.

**619** hetero-citations and *h*-index **16** (*Web of Science* – 14/11/22)

## SELECTED PUBLICATIONS

1. “The Role of Oxidation Pattern and Water Content in the Spatial Arrangement and Dynamics of Oxidized Graphene-Based Aqueous Dispersions” Anastassia Rissanou Ioannis Karnis, Fanourios Krasanakis, Kiriaki Chrissopoulou, Konstantinos Karatasos, *Int. J. Mol. Sci.*, 23 (21), 13459 (2022). (<https://doi.org/10.3390/ijms232113459>).
2. “Effects of the structure of lipid-based agents in their complexation with a single stranded mRNA fragment: a computational study” A. Rissanou, K. Karatasos, *Soft Matter*, 18, 6229-6245 (2022). (<https://doi.org/10.1039/D2SM00403H>)
3. “Polybutadiene Copolymers via Atomistic and Systematic Coarse-Grained Simulations” Rissanou, A.; Chazirakis, A., Polinska, P.; Burkhart, C.; Doxastakis, M.; Harmandaris, V. *Macromolecules*, 55 (1), 224-240 (2022). (<https://doi.org/10.1021/ma0491210>)
4. “Structure and Thermal Stability of wtRop and RM6 Proteins through All-atom Molecular Dynamics Simulations and Experiments” Maria Arnittali, Anastassia N. Rissanou, Maria Amprazi, Michael Kokkinidis, Vagelis Harmandaris, *Int. J. of Mol. Sci.*, section: *Macromolecules*, Special Issue: *Folding and Design of  $\alpha$ -Helical Proteins and Peptides: Theory Meets Nanomaterials, Biotechnology and Health*; 22(11), 5931 (2021). (DOI: [10.3390/ijms22115931](https://doi.org/10.3390/ijms22115931))
5. “Self-assembly of Alanine-Isoleucine and Isoleucine-Isoleucine Dipeptides through Atomistic Simulations and Experiments”, Anastassia N. Rissanou, Georgios Simatos, Panagiota Siachouli, Vagelis Harmandaris, Anna Mittraki, *J. Phys. Chem. B*, 124, 33, 7102–7114 (2020). (DOI: [10.1021/acs.jpcc.0c03025](https://doi.org/10.1021/acs.jpcc.0c03025))

6. "Self-Assembly of Diphenylalanine Peptides on Graphene via Detailed Atomistic Simulations" Anastassia N. Rissanou, Andriani Keliri, Maria Arnittali, Vagelis Harmandaris, **Phys. Chem. Chem. Phys.**, 22, 27645-27657 (2020). (<https://doi.org/10.1039/D0CP03671D>)
7. "Complexation of single stranded RNA with an ionizable lipid: an all-atom molecular dynamics simulation study", Anastassia N. Rissanou, Andreas Ouranidis, Kostas Karatasos, **Soft Matter** 16, 6993-7005 (2020). (<https://doi.org/10.1039/D0SM00736F>)
8. "Properties of nanographene in polymer nanocomposites through all-atom simulations: Shape fluctuations and rippling", A. N. Rissanou, P. Bacova, V. Harmandaris, **Computational Materials Science** 172, 109330 (2020). (<https://doi.org/10.1016/j.commatsci.2019.109330>)
9. "Investigation of the properties of nanographene in polymer nanocomposites through molecular simulations: dynamics and anisotropic Brownian motion", A. N. Rissanou, P. Bacova, V. Harmandaris, **Physical Chemistry Chemical Physics** 21, 23843-23854 (2019). (<https://doi.org/10.1039/C9CP02074H>)
10. "Dynamics and Structure of Monolayer Polymer Crystallites on Graphene", M. Gulde, A. N. Rissanou, V. Harmandaris, M. Mueller, S. Schäfer, and C. Ropers, **Nano Letters**, 16 (11), pp 6994–7000, (2016) (<https://doi.org/10.1021/acs.nanolett.6b03079>).
11. "Structural and Dynamical Properties of Polystyrene Thin Films Supported by Multiple Graphene Layers", Anastassia N. Rissanou and Vagelis Harmandaris, **Macromolecules**, 48 (8), 2761–2772 (2015). (<https://doi.org/10.1021/ma502524e>)
12. "Dynamics of various Polymer/Graphene Interfacial Systems through Atomistic Molecular Dynamics", Anastassia N. Rissanou and Vagelis Harmandaris **Soft Matter** 10, 2876–2888 (2014). (<https://doi.org/10.1039/C3SM52688G>)
13. "Effect of Solvent on the Self-Assembly of Dialanine and Diphenylalanine Peptides", A. N. Rissanou, E. Georgilis, E. Kasotakis, A. Mitraki and V. Harmandaris, *Journal of Physical Chemistry B* **117**(15), 3962-75 (2013) (<https://doi.org/10.1021/jp311795b>).
14. "A Monte Carlo Study of the Coil-to-Globule Transition of Model Polymer Chains near an Attractive Surface", A. N. Rissanou, S. H. Anastasiadis, I. A. Bitsanis, *Journal of Polymer Science Part B: Polym. Phys.*, **47**, 2462–2476 (2009) (<https://doi.org/10.1002/polb.21869>).
15. "Calculation of the Effect of Macromolecular Architecture on Structure and Thermodynamic Properties of Linear – Tri-Arm Polyethylene Blends from Monte Carlo Simulation", A. N. Rissanou, L. D. Peristeras, I. G. Economou *Polymer*, **48**, 3883 (2007) (<https://doi.org/10.1016/j.polymer.2007.04.066>).
16. "Monte Carlo Simulation of the Phase Behavior of Model Dendrimers", A. N. Rissanou, I. G. Economou and A. Z. Panagiotopoulos, *Macromolecules*, **39**, 6298, (2006) (<https://doi.org/10.1021/ma061339u>).