

Anastassia Rissanou

A. Peer-Reviewed Referred Journals

1. "The Information Content of Multiple Scattering Data: Monte Carlo and Laboratory Experiments",
A. N. Rissanou, S. H. Anastasiadis, I. A. Bitsanis, J. de Joannis, C. Mujat, A. Dogariu. *Prog. Colloid Polym. Sci.*, 118, 276 (2001). https://doi.org/10.1007/3-540-45725-9_58
2. "Thermal vitrification in suspensions of soft colloids: Molecular dynamics simulations and comparison with experiments",
A. N. Rissanou, D. Vlassopoulos, I. A. Bitsanis, *Phys. Rev. E*, 71, 011402 (2005).
<https://doi.org/10.1103/PhysRevE.71.011402>
3. "Temperature Induced Crystallization in Concentrated Suspensions of Multi-Arm Star Polymers: A Molecular Dynamics Study",
A. N. Rissanou, M. Yiannourakou, I. G. Economou, I. A. Bitsanis, *J. Chem. Phys.*, **124**, 044905, (2006). <https://doi.org/10.1063/1.2148964>
4. "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>
5. "A Monte Carlo Study of the Coil-to-Globule Transition of a Model Polymeric System",
A. N. Rissanou, S. H. Anastasiadis, I. A. Bitsanis *Journal of Polymer Science Part B*, **44**, 3651 (2006). <https://doi.org/10.1002/polb.21024>
6. "Amorphous and Crystalline States of Ultrasoft Colloids: A Molecular Dynamics Study",
A. N. Rissanou, M. Yiannourakou, I. G. Economou and I. A. Bitsanis, *Rheologica Acta Journal*, **46**, 755, (2007). <https://doi.org/10.1007/s00397-007-0172-0>
7. "Novel Monte Carlo Molecular Simulation Scheme Using Identity-Altering Elementary Moves for the Calculation of Structure and Thermodynamic Properties of Polyolefin Blends",
L. D. Peristeras, A. N. Rissanou, I. G. Economou and D. N. Theodorou *Macromolecules*, **40**, 2904 (2007). <https://doi.org/10.1021/ma0627121>
8. "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>

9. "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>
10. "Structure and Dynamics of Poly(methyl-methacrylate)/Graphene systems through Atomistic Molecular Dynamics Simulations",
A. N. Rissanou and V. Harmandaris, *Journal of Nanoparticle Research* **15**, 1589:1-14, (2013). <https://doi.org/10.1007/s11051-013-1589-2>
11. "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>
12. "A Molecular Dynamics Study of Polymer/Graphene Interfacial Systems",
A. N. Rissanou and V. Harmandaris *Journal of Macromolecular Symposia* **1599**, 170 (2014).
<https://doi.org/10.1063/1.4876805>
13. "Dynamics of various Polymer/Graphene Interfacial Systems through Atomistic Molecular Dynamics",
A. N. Rissanou and V. Harmandaris *Soft Matter* **10**, 2876–2888 (2014).
<https://doi.org/10.1039/C3SM52688G>
14. "Collapse Transitions in Thermosensitive Multi-block Copolymers: A Monte Carlo Study"
A. N. Rissanou, D. S. Tzeli, S. H. Anastasiadis, I. A. Bitsanis *Journal of Chemical Physics* **140**, 204904_1-13 (2014). <https://doi.org/10.1063/1.4875694>
15. "Properties of Polyethylene/Graphene Nanocomposites through Molecular Dynamics Simulations"
A. N. Rissanou, A. J. Power and V. Harmandaris, *Polymers*, **7**, 390-417 (2015).
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16. "Structural and Dynamical Properties of Polystyrene Thin Films Supported by Multiple Graphene Layers",
A. N. Rissanou and V. Harmandaris, *Macromolecules*, **48** (8), 2761–2772 (2015).
<https://doi.org/10.1021/ma502524e>
17. "Edge-functionalized Graphene as a nanofiller: Molecular Dynamics Simulation Study",
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18. "Dynamics and Structure of Monolayer Polymer Crystallites on Graphene",
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19. “Atomistic Simulation of Graphene-Based Polymer Nanocomposites”,
A. N. Rissanou, P. Bačová and V. Harmandaris, *Materials Today: Proceedings* 1736, 020015 (2016). <https://doi.org/10.1063/1.4949590>
20. “Structural and Conformational Properties of Poly(ethylene oxide)/Silica Nanocomposites: Effect of Confinement”,
A. N. Rissanou, H. Papapanou, V. S. Petrakis, M. Doxastakis, K. S. Andrikopoulos, G. A. Voyiatzis, K. Chrissopoulou, V. Harmandaris and S. H. Anastasiadis, *Macromolecules* 50 (16), 6273–6284 (2017). <https://doi.org/10.1021/acs.macromol.7b00811>
21. “Wetting Behavior of Polymer Droplets: Effects of Droplet Size and Chain Length”,
E. A. S. Evangelopoulos, A. N. Rissanou, E. Glynos, I. A. Bitsanis, S. H. Anastasiadis and V. Koutsos, *Macromolecules* 51, 2805–2816, (2018).
<https://doi.org/10.1021/acs.macromol.8b00033>
22. “Modelling of novel polymer materials through atomistic molecular dynamics simulations”,
P. Bačová, A. N. Rissanou and V. Harmandaris, *Procedia Computer Science* 136, 341-350, (2018). <https://doi.org/10.1016/j.procs.2018.08.280>
23. “Effect of macromolecular architecture on the self-assembly behavior of copolymers in a selective polymer host”,
P. Bačová, R. Foskinis, E. Glynos, A. N. Rissanou, S. H. Anastasiadis and V. Harmandaris, *Soft Matter* 14, 9562-9570 (2018). <https://doi.org/10.1039/C8SM01421C>
24. “Structure of Biomolecules Through Molecular Dynamics Simulations”,
M. Arnittali, A. N. Rissanou, V. Harmandaris, *Procedia Computer Science* 156, 69-78 (2019). <https://doi.org/10.1016/j.procs.2019.08.181>
25. “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>
26. “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, 1 109330 (2020). <https://doi.org/10.1016/j.commatsci.2019.109330>
27. “Conformations and Dynamics of Polymer Chains in Cis and Trans Poly(butadiene)/Silica Nanocomposites through Atomistic Simulations: From the Unentangled to the Entangled Regime”
A. F. Behbahani, A. Rissanou, G. Kritikos, M. Doxastakis, C. Burkhart, P. Polinska and V. Harmandaris, *Macromolecules* 53, 15, 6173–6189 (2020).
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28. “Bound Layer Polymer Behavior on Graphene and Graphene Oxide Nanosheets”
G. Kritikos, A. Rissanou, V. Harmandaris, K. Karatasos, *Macromolecules* 53, 15, 6190–6203 (2020). <https://doi.org/10.1021/acs.macromol.0c01040>
29. “Complexation of single stranded RNA with an ionizable lipid: an all-atom molecular dynamics simulation study”,
A. N. Rissanou, A. Ouranidis, Kostas. Karatasos, *Soft Matter* 16, 6993-7005 (2020).
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30. “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). <https://doi.org/10.1021/acs.jpcc.0c03025>
31. “Self-Assembly of Diphenylalanine Peptides on Graphene via Detailed Atomistic Simulations”
A. N. Rissanou, A. Keliri, M. Arnittali, V. Harmandaris, *Phys. Chem. Chem. Phys.*, 22, 27645-27657 (2020). <https://doi.org/10.1039/D0CP03671D>
32. “Dynamics and Rheology of Polymer Melts via Hierarchical Atomistic, Coarse-grained, and Slip-spring Simulations”
A. Behbahani, L. Schneider, A. Rissanou, A. Chazirakis, P. Bačová, P. Kumar Jana, W. Li, M. Doxastakis, P. Polińska, C. Burkhardt, M. Müller, and V. A. Harmandaris
Macromolecules 54, 6, 2740–2762 (2021). <https://doi.org/10.1021/acs.macromol.0c02583>
33. “Structure and Thermal Stability of wtRop and RM6 Proteins through All-atom Molecular Dynamics Simulations and Experiments”
M. Arnittali, A. N. Rissanou, M. Amprazi, M. Kokkinidis, V. Harmandaris, *International Journal of Molecular Sciences*, section: *Macromolecules*, Special Issue: *Folding and Design of α -Helical Proteins and Peptides: Theory Meets Nanomaterials, Biotechnology and Health*; *Int. J. Mol. Sci.* 22(11), 5931 (2021). <https://doi.org/10.3390/ijms22115931>
34. “Polybutadiene Copolymers via Atomistic and Systematic Coarse-Grained Simulations”
A. Rissanou, A. Chazirakis, P. Polinska, C. Burkhardt, M. Doxastakis, V. Harmandaris,
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35. “Effects of the structure of lipid-based agents in their complexation with a single stranded mRNA fragment: a computational study”
A. N. Rissanou, K. Karatasos, *Soft Matter* 18, 6229-6245 (2022).
<https://doi.org/10.1039/D2SM00403H>

36. “Dynamics of Polymer Chains in Poly(ethylene oxide)/Silica Nanocomposites via a Combined Computational and Experimental Approach”
A. J. Power, H. Papananou, A. N. Rissanou, M. Labardi, K. Chrissopoulou, V. Harmandaris and S. H. Anastasiadis, *J. Phys. Chem B*, 126, 39, 7745–7760 (2022).
<https://doi.org/10.1021/acs.jpcc.2c04325>
37. “The Role of Oxidation Pattern and Water Content in the Spatial Arrangement and Dynamics of Oxidized Graphene-Based Aqueous Dispersions”
A. Rissanou I. Karnis, F. Krasanakis, K. Chrissopoulou, K. Karatasos, *Int. J. Mol. Sci.*, 23 (21), 13459 (2022). <https://doi.org/10.3390/ijms232113459>

B. Book Chapters

1. “Mesoscopic Simulations of T-Induced Solidification in Dense Suspensions of Ultrasoft Supramolecules”
I. A. Bitsanis, A. N. Rissanou, M. Yannourakou, I. G. Economou, D. Vlassopoulos
Lecture Series on Computer and Computational Sciences ICCMSE 2006, Chania, Crete, Greece. Volume 6, 2006, p. 1:4 (2006).
2. “Conformational Transitions of a Model Polymeric System near Attractive Surfaces: A Monte Carlo Study”
A. N. Rissanou, I. A. Bitsanis, S. H. Anastasiadis
International Conference of Computational Methods in Sciences and Engineering 2007 (ICCMSE 2007) Corfu, Kerkyra, Greece. American Inst. of Physics Proceedings (T. E. Simos and G. Maroulis, Eds.), Vol. 963, pp. 428-431 (2007).