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ResearcherID: [O-4544-2018](https://pubs.acs.org/doi/10.26434/chemrxiv-2018-04544)

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EDUCATION

- **PhD:** "[Atomistic and mesoscopic simulations of the interfacial dynamics of polymer melts](#)", School of Chemical Engineering, NTUA, Athens, Greece.
- **MSc:** "[Single layer and multilayer graphene under compression](#)" Graduate Program in Materials Science and Engineering, NTUA, Athens, Greece.
- **BSc:** "Investigation of the effect of point defects in the phononic spectrum of graphene" Department of Material Science, UoP, Patras, Greece.

RESEARCH APPOINTMENTS

- | | |
|-------------------|--|
| 01/2024 – now | Associate Researcher (C), TCPI/NHRF, Athens, Greece. |
| 09/2019 – 12/2024 | Postdoctoral Researcher, School of Chemical Engineering, NTUA, Athens, Greece. |
| 11/2014 – 05/2015 | Assistant Researcher, FORTH /ICE-HT, Patras, Greece. |
| 02/2014 – 06/2015 | Assistant Researcher, Department of Material Science, UoP, Patras, Greece. |

MAIN RESEARCH INTERESTS

- **Multiscale modelling of materials:** Addressing atomistic (*Ab-Initio*, *MD* & *MC*), and mesoscopic scales, the latter incorporating particle-based (*DPD* and *CGMD*), field-theoretic (*SCFT*, *Phase-field*), and hybrid particle-field (*lattice*, *kernels*) approaches.
- **Force-field optimization:** Atomistic and mesoscopic models via *Boltzmann-inversion*, *Bayesian optimization*, and *machine-learning* strategies.

- **2D Materials:** Thermal transport, stability and mechanics.
- **Polymers:** thermodynamics of polymers in proximity to *vacuum*, *polymer* and *solid* interfaces; rheology, slip and fracture phenomena
- **Nanocomposites:** optimal design of polymer-matrix nanocomposites by introducing functionalized NPs or thermoplastic polymers.
- **Scientific software:** Development of simulation packages, algorithms, and post-processing tools.

EXTERNAL FUNDING

- Modeling reaction-induced phase separation for the production of thermoplastic-toughened thermosets. Syensqo, USA. Collaborating Researcher. (11/2023-12/2024)
- Coarse-grained Modeling Investigations of Polymer Adhesion for Solid State Batteries. SOLVAY, Italy. Collaborating Researcher. (12/2021-11/2023)
- Multiscale Modeling for the Design of Antifouling Copolymers. SOLVAY, France. Collaborating Researcher. (09/2019-05/2021)
- Multiscale Simulations of Soft Matter Systems, GSRT, Project Σ2006Σ01330025. Collaborating Researcher. (05/2018-12/2018)
- Multiscale Simulations of Complex Polymer Systems (MUSICOMPS). LIMMAT FOUNDATION, Zurich, Switzerland. Collaborating Researcher. (08/2015-06/2019)
- Thales – Graphene and nanocomposite Materials: manufacture, properties and applications. GRAPHENE FLAGSHIP, MIS380389. (11/2014-04/2015)
- Surface treatment of multicrystalline Silicon solar cells for improved efficiency (STSSoC). SYNERGASIA and GSRT. Collaborating Researcher. (02/2014-06/2015)

HONNORS AND AWARDS

- IAKOVOS GIOUROULIAN for my PhD dissertation (2020).
- DIMITRIS N. CHORAFAS, for the best PhD dissertation in NTUA. (2019).
- THOMAIDIO AWARD for publications (2018-2019).
- Thales scholarship for Master's Students (11/2014-04/2015).

PROFESSIONAL AFFILIATIONS & ACTIVITIES

- Reviewer in over 20 Journals (86 [verified](#) reviews).
- Reviewer Panel, Polymers.
- System administrator @ COMSE group (2018-2024).
(GLASS cluster; CentOS release 6.3, 17 nodes, ~300 cores).

PUBLICATIONS - PRESENTATIONS

- 35 articles in peer-reviewed journals, 4 articles in referred international conference proceedings
- 39 documents, 485 citations by 330 documents, h-index 13 ([Web of Science](#), January 2025)
- 4 invited talks/workshops, 14 contributions to international conferences
- 9 contributions to national conferences
- Co-supervised 8 BSc and 4 MSc students
- 1 patent

SELECTED RECENT PUBLICATIONS

1. "Development of a Meshless kernel-based Scheme for Particle-Field Brownian Dynamics Simulations", A. P. Sgouros, D. N. Theodorou, [J. Phys. Chem. B **128**, 6907 \(2024\)](#).
2. "Buckling kinetics of graphene membranes under uniaxial compression", A. P. Sgouros, E. Drougkas, S. V. Kallivokas, D.N. Theodorou, [Physical Review E **104**, 23001 \(2024\)](#).
3. "Tailoring Nanoparticle Orientation in Polymer Matrices via Nonuniform Grafting: Implications for Nanoparticle Dispersions and Self-Assembled Nanocomposite Morphologies" C. J. Revelas, A. P. Sgouros, A. T. Lakkas, D. N. Theodorou, [ACS Appl. Nano Mater. **7**, 19329 \(2024\)](#).
4. "Delayed Thermal Relaxation in Lateral Heterostructures of Transition-Metal Dichalcogenides", N. Kanistras, A. P. Sgouros, G. Kalosakas, M. M. Sigalas, [J. Phys. Chem. C **126**, 15, 6815 \(2022\)](#).
5. "Multiscale simulations of polyzwitterions in aqueous bulk solutions and brush array configurations", A. P. Sgouros, S. Knippenberg, M. Guillaume, D. N. Theodorou, [Soft Matter **17**, 10873 \(2021\)](#).
6. "Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory", A. P. Sgouros, C. J. Revelas, A. T. Lakkas, D. N. Theodorou, [Polymers **13**, 1197 \(2021\)](#).
7. "Effect of Surface Nanopatterning on Slip: The Case of Couette Flow of Long-Chain Polyethylene Melt Flowing Past Gold Surfaces", A. P. Sgouros, D. S. Tsagkalakis, D. N. Theodorou, [J. Phys. Chem. B **125**, 6681 \(2021\)](#).
8. "Efficient Mechanical Stress Transfer in Multilayer Graphene with a Ladder-like Architecture", A. P. Sgouros, C. Androulidakis, G. Tsoukleri, G. Kalosakas, N. Delikoukos, S. Signetti, N. M. Pugno, J. Parthenios, C. Galiotis, K. Papagelis, [Appl. Mater. Interfaces **13**, 4473 \(2021\)](#).

9. "Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites", S. V. Kallivokas, A. P. Sgouros, D.N. Theodorou, [Physical Review E - Rapid Communications **102**, 30501 \(2020\)](#).
10. "Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment", A. P. Sgouros, G. G. Vogiatzis, G. Megariotis, C. Tzoumanekas, D. N. Theodorou, [Macromolecules **52**, 7503 \(2019\)](#).
11. "Temperature profiles and thermal conductivities of nanostructured transition metal dichalcogenides", A. P. Sgouros, S. Konstantopoulou, G. Kalosakas, M. M. Sigalas, [Int. J. Heat Mass Transf. **140**, 579 \(2019\)](#).
12. "Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies", A. P. Sgouros, G. G. Vogiatzis, G. Kritikos, A. Boziki, A. Nikolakopoulou, A. Liveris, D. N. Theorodou, [Macromolecules **50**, 8827 \(2017\)](#).
13. "Uniaxial Compression of suspended single and multilayer graphenes", A. P. Sgouros, G. Kalosakas, C. Galiotis, K. Papagelis, [2D Mater. **3**, 025033 \(2016\)](#).
14. "Nanoscale Phononic Interconnects in THz frequencies", A. P. Sgouros, M. R. Neupane, M. M. Sigalas, A. Aravantinos-Zafiris, R. K. Lake, [RSC PCCP **16**, 23355 \(2014\)](#).