Aristotelis P. SGOUROS

Publications (January 2025)

A. Peer-reviewed journals

A1. **Sgouros, A.P.***; Michos, F. I.; Sigalas, M. M.; Kalosakas G. "Thermal Relaxation in Janus Transition Metal Dichalcogenide Bilayers." *Materials*, **2024**, 17, 4200.
DOI: 10.3390/ma17174200

A2. Revelas, C.J.‡; **Sgouros, A.P.‡**; Lakkas, A.T.; Theodorou, D. N.* "Tailoring Nanoparticle Orientation in Polymer Matrices via Nonuniform Grafting: Implications for Nanoparticle Dispersions and Self-Assembled Nanocomposite Morphologies." *ACS Appl. Nano Mater.*, **2024**, 7, 16, 19329.
DOI: 10.1021/acsanm.4c03229

A3. **Sgouros, A.P.***; Theodorou, D.N. "Development of a Meshless kernel-based Scheme for Particle-Field Brownian Dynamics Simulations." *J. Phys. Chem.* B **2024**, 128, 28, 6907.
DOI: 10.1021/acs.jpcb.4c01441

A4. **Sgouros, A.P.***; Drougkas, E.; Kallivokas, S.V.; Theodorou, D.N. "Buckling kinetics of graphene membranes under uniaxial compression." *PRE*, **2024**, 104, 23001.
DOI: 10.1103/PhysRevE.109.L023001

A5. Revelas, C.J.‡; **Sgouros, A.P.‡**; Lakkas, A.T.; Theodorou, D.N.* "Addressing Nanocomposite Systems via 3D-SCFT: Assessment of Smearing Approximation and Irregular Grafting Distributions." *Macromolecules* **2023**, 56, 1731.
DOI: 10.1021/acs.macromol.2c02474

A6. **Sgouros, A.P.***; Theodorou, D.N.*"Addressing the Folding of Intermolecular Springs in Particle Simulations: Fixed Image Convention." *Computation* **2023**, 11, 106
DOI: 10.3390/computation11060106

A7. **Sgouros, A.P.‡**; Revelas, C.J.‡; Lakkas, A.T.; Theodorou, D.N.* "Solvation Free Energy of Dilute Grafted (Nano)particles in Polymer Melts via Self-Consistent Field Theory." *J. Phys. Chem.* B **2022**, 126, 38, 7454.
DOI: 10.1021/acs.jpcb.2c05306

A8. Kanistras, N.‡; **Sgouros, A.P.‡**; Kalosakas, G.; Sigalas, M.M.* "Delayed Thermal Relaxation in Lateral Heterostructures of Transition-Metal Dichalcogenides." *J. Phys. Chem.* C **2022**, 126, 15, 6815.
DOI: 10.1021/acs.jpcc.2c00789

A9. **Sgouros, A.P.**; Knippenberg, S.; Guillaume, M.; Theodorou, D.N.* "Multiscale simulations of polyzwitterions in aqueous bulk solutions and brush array configurations." Soft Matter **2021**, 17, 10873.
DOI: 10.1039/d1sm01255j

A10. Revelas, C.J.‡; **Sgouros, A.P.*‡**; Lakkas, A.T.; Theodorou, D.N.* "RuSseL : A Self-Consistent Field Theory Code for Interphases, Inhomogeneous Polymer." *Computation* **2021**, 9, 57.
DOI: 10.3390/computation9050057

A11. **Sgouros, A.P.*‡**; Revelas, C.J.‡; Lakkas, A.T.; Theodorou, D.N.* "Potential of Mean Force between Bare or Grafted Silica/Polystyrene Surfaces from Self-Consistent Field Theory." *Polymers* **2021**, 13, 1197.
DOI: 10.3390/polym13081197

A12. Lakkas, A.T.[‡]; **Sgouros, A.P.**[‡]; Revelas, C.J.[‡]; Theodorou, D.N.* "Structure and Thermodynamics of Grafted Silica/Polystyrene Nanocomposites Investigated Through Self-Consistent Field Theory." *Soft Matter* **2021**, 17, 4077–4097.
DOI: 10.1039/D1SM00078K

A13. **Sgouros, A.P.**; Tsagkalakis, D.S.; Theodorou, D.N.* "Effect of Surface Nanopatterning on Slip : The Case of Couette Flow of Long-Chain Polyethylene Melt Flowing Past Gold Surfaces." *J. Phys. Chem.* B **2021**, 125, 6681–6696.
DOI: 10.1021/acs.jpcb.1c02546

A14. **Sgouros, A.P.**; Karantagli, E.; Sigalas, M.M.* "Reflectivity Reduction of Nanopatterned c-Si Solar Cells with Antireflective Coatings Exposed to a Wide Range of Incidence Angles." *Photonics Nanostructures - Fundam. Appl.* **2021**, 43, 100893.
DOI: 10.1016/j.photonics.2020.100893

A15. **Sgouros, A.P.**; Androulidakis, C.; Tsoukleri, G.; Kalosakas, G.; Delikoukos, N.; Signetti, S.; Pugno, N.M.; Parthenios, J.; Galiotis, C.; Papagelis, K.* "Efficient Mechanical Stress Transfer in Multilayer Graphene with a Ladder-like Architecture." *Appl. Mater. Interfaces* **2021**, 13, 4473–4484.
DOI: 10.1021/acsami.0c18774

A16. Kallivokas, V.S.[‡]; **Sgouros, A.P.**[‡]; Theodorou, D.N.* "Kinetic concepts and local failure in the interfacial shear strength of epoxy-graphene nanocomposites." *PRE – Rapid Communications*, **2020**, 102, 30501.
DOI: 10.1103/PhysRevE.102.030501

A17. Simavilla, N.D.; **Sgouros, A.P.**; Vogiatzis, G.G.; Tzoumanecas, C.; Georgilas, V.; Verbeeten, M.H.W; Theodorou, D. N.* "A Molecular Dynamics Test of the Stress-Thermal Rule in Polyethylene and Polystyrene Entangled Melts." *Macromolecules*, **2020**, 53, 789-802.
DOI: 10.1021/acs.macromol.9b02088

A18. **Sgouros, A.P**; Theodorou, D.N.*; "Atomistic Simulations of Long-Chain Polyethylene Melts Flowing Past Gold Surfaces: Structure and Wall-Slip." *Molecular Physics* **2020**, 118, 1706775.
DOI: 10.1080/00268976.2019.1706775

A19. **Sgouros, A.P.**; Vogiatzis, G.G.; Megariotis, G.; Tzoumanekas, C.; Theodorou, D.N.* "Multiscale Simulations of Graphite-Capped Polyethylene Melts: Brownian Dynamics/Kinetic Monte Carlo Compared to Atomistic Calculations and Experiment." *Macromolecules*, **2019**, 52, 7503-7523.
DOI: 10.1021/acs.macromol.9b01379

A20. Lakkas, A.T.; **Sgouros, A.P.**; Theodorou, D.N.*; "Self-Consistent Field Theory Coupled with Square Gradient Theory of Free Surfaces of Molten Polymers and Compared to Atomistic Simulations and Experiment." *Macromolecules*, **2019** 52, 5337-5356.
DOI: 10.1021/acs.macromol.9b00795

A21. **Sgouros, A.P.**[‡]; Konstantopoulou, S.[‡]; Kalosakas, G.; Sigalas, M.M.*; "Temperature profiles and thermal conductivities of nanostructured transition metal dichalcogenides." *Int. J. Heat Mass Transf.*, **2019** 140, 579-586.
DOI: 10.1016/j.ijheatmasstransfer.2019.06.026

A22. Kallivokas, V.S.; **Sgouros, A.P.**; Theodorou, D.N.* "Molecular Dynamics Simulations of EPON-862/DETDA Epoxy Networks: Structure, Topology, Elastic Constants, and Local Dynamics." *Soft Matter*, **2019**, 15, 721-733.
DOI: 10.1039/C8SM02071J

A23. **Sgouros, A.P.**; Lakkas, A.T.; Megariotis, G.; Theodorou, D.N.* "Mesoscopic Simulations of Free Surfaces of Molten Polyethylene: Brownian Dynamics/Kinetic Monte Carlo Coupled with Square Gradient Theory and Compared to Atomistic Calculations and Experiment." *Macromolecules*, **2018**, 51, 9798-9815.
DOI: 10.1021/acs.macromol.8b01873

A24. Megariotis, G.; Vogiatzis, G.; **Sgouros, A.P.**; Theodorou, D.N.* "Slip Spring-Based Mesoscopic Simulations of Polymer Networks: Methodology and the Corresponding Computational Code." *Polymers*, **2018**, 10, 1156. DOI: 10.3390/polym10101156

A25. **Sgouros, A.P.**; Kalosakas, G.; Papagelis, K.; Galiotis, C.* "Compressive response and buckling of graphene nanoribbons." *Sci. Rep.* **2018**, 8, 9593. DOI: 10.1038/s41598-018-27808-0

A26. **Sgouros, A.P.**; Vogiatzis, G.G.; Kritikos, G.; Boziki, A.; Nikolakopoulou, A.; Liveris, D.; Theodorou, D.N.* "Molecular Simulations of Free and Graphite Capped Polyethylene Films: Estimation of the Interfacial Free Energies." *Macromolecules*, **2017**, 50, 8827-44. DOI: 10.1021/acs.macromol.7b01808

A27. **Sgouros, A.P.**; Megariotis, G.; Theodorou, D.N.* "Slip-spring model for the Linear and Nonlinear Viscoelastic Properties of Molten Polyethylene Derived from Atomistic Simulations." *Macromolecules*, **2017**, 50, 4524-41. DOI: 10.1021/acs.macromol.7b00694

A28. Konstantopoulou, A.; **Sgouros, A.P.**; Sigalas, M.M.* "Computational Study of Phononic resonators and waveguides in monolayer transition metal dichalcogenides." *RSC PCCP*, **2017**, 19, 8082-8090. DOI: 10.1039/C7CP00155J

A29. Michos, F. I.; **Sgouros, A.P.**; Sigalas, M. M.* "Ab initio study of Boron and Aluminum Hydrides nanoparticles." *Int. J. Hydrog. Energy*, **2016**, 41, 20210-16. DOI: 10.1016/j.ijhydene.2016.09.011

A30. **Sgouros, A.P.**; Kalosakas, G.; Galiotis, C.; Papagelis, K. "Uniaxial Compression of suspended single and multilayer graphenes." *2D Mater*. **2016**, 3, 025033. DOI: 10.1088/2053-1583/3/2/025033

A31. Koukaras, E.N.; **Sgouros, A.P.**; Sigalas, M.M.* "Fully Hydrogenated Beryllium Nanoclusters." *J. Am. Chem. Soc*, **2016**, 138, 3218-3227. DOI: 10.1021/jacs.6b00135

A32. **Sgouros, A.P.**; Sigalas, M.M.* "Nanoscale Phononic Waveguides and Resonators in the <111> surface of 3C-GeSi." *J. Surf. Interf.*, **2015**, 138, 3218-3227. DOI: 10.1166/jsim.2015.1078

A33. **Sgouros, A.P.**; Kalosakas, G.; Sigalas, M.M.; Papagelis, K.* "Exotic carbon nanostructures obtained through controllable defect engineering." *RSC adv*. **2015**, 5, 39930-39937. DOI: 10.1039/C5RA04831A

A34. **Sgouros, A.P.**; Neupane, M.R.; Sigalas, M.M.*; Aravantinos-Zafiris, A.; Lake, R.K. "Nanoscale Phononic Interconnects in THz frequencies." *RSC PCCP*, **2014**, 16, 23355-64. DOI: 10.1039/C4CP02328E

A35. **Sgouros, A.P.**; Sigalas, M.M.; Papagelis, K.; Kalosakas, G.* "Transforming graphene nanoribbons to nanotubes by use of point defects." *J. Phys.: Condens. Matt.* **2014**, 26, 125301. DOI: 10.1088/0953-8984/26/12/125301

A36. **Sgouros, A.P.**; Sigalas, M.M.*; Kalosakas, G.; Papagelis, K.; Papanicolaou, N.I. "Phononic band gap engineering in graphene." *J. Appl. Phys.* **2012**, 112, 094307. DOI: 10.1063/1.4763479

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B. Refereed Proceedings

B1. Philippas, A.P.; **Sgouros, A.P.**, Megariotis, G.; Theodorou, D.N.* "Mesoscopic Simulations of Star Polyethylene Melts at Equilibrium and under Steady Shear Flow." *AIP Conf. Proc.* **2021**, 2343, 130003.
DOI: 10.1063/5.0047757

B2. Revelas, C.J.; **Sgouros, A.P.**; Lakkas, A.T.; Theodorou, D.N.* "A Three-Dimensional Finite Element Methodology for Addressing Heterogeneous Polymer Systems with Simulations Based on Self-Consistent Field Theory." *AIP Conf. Proc.* **2021**, 2343, 130002.
DOI: 10.1063/5.0047729

B3. Evangelou, N.; Megariotis, G.; **Sgouros, A.P.**; Vogiatzis, G.G.; Romanos A. Nikolaos; Theodorou, D.N.* "Coarse-Grained Simulations of Bidisperse Polymer Melts." *AIP Conf. Proc.* **2021**, 2343, 130008.
DOI: 10.1063/5.0047764

B4. Kritikos, G.*; **Sgouros, A.P.**; Vogiatzis, G.G.; Theodorou, D.N. "Molecular Dynamics Study of Polyethylene under Extreme Confinement." *J. Phys. Conf. Ser*. **2016**, 732, 012012.
DOI: 10.1088/1742-6596/738/1/012012