Anastasios Gkotzias

Scientific publications under the name: Anastasios Gotzias

N.C.S.R. 'Demokritos'
Institute of Nanoscience Nanotechnology
Department of Physical Chemistry
Agia Paraskevi, Athhens, Greece
Phone (m): (0030) 6974 34 92 88

Email: a.gotzias@inn.demokritos.gr
ORCID ID: 0000-0002-0823-0703
Demokritos (Homepage)
Social: ResearchGate
GitHub

Education

1993-1999 Chemical Engineering, University of Patras.

2005-2006 Master, Inter- Departmental Postgraduate program *Computational Mechanics*.
School of Chemical Engineering, National Technical University of Athens (NTUA) .
Thesis:
Heuristics for the solution of the Bin Packing Problem

2007-2012 PhD, School of Sciences and Engineering,
Chemistry Department, University of Crete.
Thesis:
Study of hydrogen adsorption in nano-structured carbon materials, with a combination of experimental methods and Monte Carlo simulations.

Professional experience

2017- Researcher at the Institute of Nanoscience & Nanotechnology
NCSR Demokritos.

2007-2017 Research Personnel at NCSR Demokritos.

2006-2007 Chemical Engineer R&D at the INASCO company.

2002-2006 Research associate in the Membranes for Environmental separations Laboratory
of Institute of Physical Chemistry Institute of NCSR Demokritos.
Funded by research projects with the supervision of dr. N. Kanellopoulos.

Research objective

Molecular simulation methods in porous solids:
My research focuses on advancing the molecular-level understanding of gas and liquid adsorption in porous and solid materials using state-of-the-art molecular simulation techniques. I aim to bridge theoretical and experimental approaches by fostering collaboration across academia, industry, and innovation-focused startups. The scope of my work is intentionally broad, addressing a wide variety of adsorbed species—including gases, liquids, ions, and biomolecules—and diverse host materials, from organic and inorganic solids to hybrid frameworks and natural porous media.

Research Collaborations / International Networks

COST Action CA22147 – EU4MOFs (European Metal-Organic Framework Network). Role: Member of Working Group 4 – MOF Computational Tools and Machine Learning. Focus: Contributing expertise in molecular simulations and digital workflows to support MOF discovery, property prediction, and data-driven design across European labs. Duration: 2025 – Present

COST Action CA23111 – SNOOPY: Searching for Nanostructured or pOre fOrming Peptides for therapY. Role: Member of Working Groups 1 & 2: WG1 – Computational Methods for Assessment of Peptides and Peptide Nanostructures, WG2 – Production and Characterization of Bioactive Peptides and Peptide Nanostructures. Focus: Contributing member with expertise in molecular simulations of peptide assemblies and structure–function prediction. Supporting the integration of computational insights into experimental design and therapeutic evaluation. Duration: 2025 – Present

Research interests and skills

I have developed an efficient computational workflow tailored for free energy simulations, enabling accurate calculation of binding energies in complex molecular systems. This approach is particularly suited for layered materials—such as graphene oxides, metal oxides, or nanosheets—as well as host–guest systems involving the adsorption of gases, drugs, or peptides within porous solids.

I investigate the biocompatibility of carbon-based materials by modeling how carbon nanoparticles replicate the transport properties and binding affinities of proteins and other biomolecules. Additionally, I examine their interactions with cholesterol-rich components found in membrane bilayers.

I use Grand Canonical Monte Carlo (GCMC) simulations to study quantum sieving effects in nanoscale confinements. For hydrogen interactions, I apply the Feynman–Hibbs (FH) potential, which provides a simplified yet effective way to account for the quantum behavior of light molecules like hydrogen, while remaining computationally efficient. To my knowledge, no other GCMC simulation package currently includes the FH potential, making this implementation unique.

I developed a software tool for building molecular models of carbon nanohorns—nanotube-like structures capped with sharp conical tips. These nanohorns can have five distinct tip angles, depending on the number of pentagonal carbon rings (from one to five) near the apex, which create the necessary surface curvature. The tool can generate models containing up to 10,000 carbon atoms, with hydrogen atoms added at the edges. All output files are fully compatible with GROMACS simulation modules.

I develop simulation models that explicitly account for the oxygen content on carbon surfaces, treating it as a key factor in surface heterogeneity during molecular adsorption. These parameterized simulations help interpret the surface chemistry of oxidized graphites and graphene nanosheets, based on gas adsorption data from carbon samples. This approach has proven to be more accurate and efficient than standard analysis methods available in commercial instrument software.

Codes developed

Hycones software: A specialized molecular simulation code for predicting H_2 sorption isotherms on single-angle carbon cones across varying pressures and temperatures. It integrates Feynman–Hibbs quantum corrections and uses path integral Monte Carlo to simulate light adsorbates. The code uniquely includes a routine for generating multilayered carbon cones and disks of any size with accurate bonding. It also supports competitive adsorption of gas mixtures and is currently being redesigned for parallel computing.

Auto_ Rubo routine: This module performs sequential calibration and tare operations for a gravimetric analyzer, integrated in real-time with LabView. It corrects for sample buoyancy affected by pressure and temperature changes, estimates equilibration time, and predicts the final adsorbate mass.

IAST solution: This solution algorithm calculates the competitive adsorption behavior of gaseous mixtures, regardless of the number of adsorbate components. It uses analytical expressions with fitting parameters to describe the pure component isotherms.

T-IAST (Temperature-Dependent IAST): A temperature-responsive extension of IAST designed to compute multicomponent gas adsorption in porous materials at variable temperatures. T-IAST integrates easily with commercial gas adsorption instruments.

Pore Size regularization: This method extracts a distribution function from desorption isotherms using Tikhonov regularization and a truncated SVD solver, capturing porous solid heterogeneity. It can also support machine learning models for screening adsorption performance.

Density splitter: This post-processing tool analyzes GCMC simulations by dividing a cylindrical pore into concentric intervals (δr) and computing the particle count $N(r)$ in each, yielding the averaged adsorbate density distribution.

Multiplot generator: This application creates arrays of multi-panel graphs or insets, allowing users to define panel count, layout, plot quantity per graph, legends, and axis settings. It is implemented using Bash and Gnuplot.

High performance computing projects, (HPC)

The following projects refer to the access in the High Performance Computing Services of the Greek National Infrastructure for Research and Technology, GRNET-ARIS.

1st pilot call, *DISCO*, Diffusion in Stratum Corneum. Computing time earned: 5×10^3 hours (2016).

5th pilot call, *Bio-Salt*, Bio membranes for desalination. Computing time earned: 3×10^5 hours (2018).

7th & 9th pilot calls, *WATCH*, Water channels in lipid membranes. Computing time earned: 5×10^5 hours (2019 & 2020).

11th pilot call, *INJECT*, Injecting carbon nanoparticles in living cells . Computing time earned: 5×10^6 hours (2021).

14th and 16th pilot calls, *ADSORB*, Removal of antibiotics from aqueous solutions using carbon adsorbents, Computing time earned: 1×10^7 hours (2022-2025).

Programming languages and tools

Programming Languages: Fortran, Matlab, Bash, Python, Gnuplot, Matplotlib, LaTeX, LabVIEW, Emacs Lisp, Perl, C++.

Simulation Packages: GROMACS, MuSiC, RASPA, MCCCS Towhee, DL_ POLY & DL_ MONTE, PovRay, VMD.

Instrumentation: N_2 Porosimeter, HyEnergy, custom gravimetric balances, Rubotherm, Thermal desorption mass spectrometry, Raman Spectroscopy.

Miscellaneous

Certified reviewer in Publons.

Member of the American Chemical Society (ACS) and the International Adsorption Society (IAST)

Secretary at the scientific council of Physical Chemistry Institute (i.e., INN) of Demokritos. Writing minutes, proceedings, and decisions of the Council's monthly meetings. Volunteer (2008-2011)

Editor at GFOSS - Open Technologies Alliance (2016-today).

Publications

Book Chapters

1 M. Konstantakou, A. Gotzias, M. Kainourgiakis, A. K. Stubos, and T. A. Steriotis. GCMC Simulations of Gas Adsorption in Carbon Pore Structures. In *Applications of Monte Carlo Method in Science and Engineering* S. Mordechai, Ed. InTech, 2011

2 G. Karataraki, A. Gotzias, Elena Tocci. Carbon Molecular Models for Desalination. In *Membrane Desalination* Boca Raton, Ed. CRC Press, 2021

Refereed Journal Papers

3 K.A. Stoitsas, A. Gotzias, E.S. Kikkinides, Th.A. Steriotis, N.K. Kanellopoulos, M. Stoukides, and V.T. Zaspalis. Porous ceramic membranes for propane-propylene separation via the π-complexation mechanism: Unsupported systems. *Microporous and Mesoporous Materials*, 78(2-3):235 – 243, 2005

4 A. Gotzias, H. Heiberg-Andersen, M. Kainourgiakis, and Th. Steriotis. Grand canonical monte carlo simulations of hydrogen adsorption in carbon cones. *Applied Surface Science*, 256(17):5226 – 5231, 2010

5 A. Gotzias, H. Heiberg-Andersen, M. Kainourgiakis, and Th. Steriotis. A grand canonical monte carlo study of hydrogen adsorption in carbon nanohorns and nanocones at 77 k. *Carbon*, 49(8):2715 – 2724, 2011

6 A. Gotzias, E. Tylianakis, G. Froudakis, and Th. Steriotis. Theoretical study of hydrogen adsorption in oxygen functionalized carbon slit pores. *Microporous and Mesoporous Materials*, 154:38 – 44, 2012

7 A. Gotzias and Th. Steriotis. D 2/h 2 quantum sieving in microporous carbons: A theoretical study on the effects of pore size and pressure. *Molecular Physics*, 110(11-12):1179 – 1187, 2012

8 A. Gotzias, G. Charalambopoulou, A. Ampoumogli, I. Krkljus, M. Hirscher, and Th. Steriotis. Experimental and theoretical study of d2/h2 quantum sieving in a carbon molecular sieve. *Adsorption*, 19(2-4):373 – 379, 2013

9 A. Gotzias, E. Tylianakis, G. Froudakis, and Th. Steriotis. Effect of surface functionalities on gas adsorption in microporous carbons: A grand canonical monte carlo study. *Adsorption*, 19(2-4):745 – 756, 2013

10 Ivana Krkljus, Theodore Steriotis, Georgia Charalambopoulou, Anastasios Gotzias, and Michael Hirscher. H2/d2 adsorption and desorption studies on carbon molecular sieves with different pore structures. *Carbon*, 57:239 – 247, 2013

11 K. Vasanth Kumar, G. Charalambopoulou, M. Kainourgiakis, A. Gotzias, A. Stubos, and Th. Steriotis. The required level of isosteric heat for the adsorptive/storage delivery of h2in the uio series of mofs. *RSC Advances*, 4(85):44848 – 44851, 2014

12 A. Gotzias, E. Tylianakis, G. Froudakis, and Th. Steriotis. Adsorption in micro and mesoporous slit carbons with oxygen surface functionalities. *Microporous and Mesoporous Materials*, 209:141 – 149, 2015

13 Anastasios Gotzias, Georgia Charalambopoulou, and Theodore Steriotis. On the orientation of n2 and co2 molecules adsorbed in slit pore models with oxidised graphitic surface. *Molecular Simulation*, 42(3):186 – 195, 2016

14 Anastasios Gotzias. The effect of gme topology on multicomponent adsorption in zeolitic imidazolate frameworks. *Physical Chemistry Chemical Physics*, 19(1):871 – 877, 2017

15 Anastasios Gotzias, Michael Kainourgiakis, and Athanassios Stubos. Enhanced co 2 selectivity within the cavity of gmelinite frameworks. *Adsorption*, 24(4):371 – 379, 2018

16 Anastasios Gotzias, Evangelos Kouvelos, and Andreas Sapalidis. Computing the temperature dependence of adsorption selectivity in porous solids. *Surface and Coatings Technology*, 350:95 – 100, 2018

17 Anastasios Gotzias. Calculating adsorption isotherms using lennard jones particle density distributions. *Journal of Physics Condensed Matter*, 31(43), 2019

18 Georgia Karataraki, Andreas Sapalidis, Elena Tocci, and Anastasios Gotzias. Molecular dynamics of water embedded carbon nanocones: Surface waves observation. *Computation*, 7(3), 2019. All Open Access, Gold Open Access

19 Ioannis N. Floros, Evangelos P. Kouvelos, Georgios I. Pilatos, Evangelos P. Hadjigeorgiou, Anastasios D. Gotzias, Evangelos P. Favvas, and Andreas A. Sapalidis. Enhancement of flux performance in ptfe membranes for direct contact membrane distillation. *Polymers*, 12(2), 2020. All Open Access, Gold Open Access, Green Open Access

20 Anastasios Gotzias and Andreas Sapalidis. Pulling simulations and hydrogen sorption modelling on carbon nanotube bundles. *C*, 6(1), 2020

21 Athanassios G. Kontos, George Em. Romanos, Charitomeni M. Veziri, Anastasios Gotzias, Michalis K. Arfanis, Evangelos Kouvelos, Vlassis Likodimos, Georgios N. Karanikolos, and Polycarpos Falaras. Correlating vibrational properties with temperature and pressure dependent co2 adsorption in zeolitic imidazolate frameworks. *Applied Surface Science*, 529, 2020

22 Anastasios Gotzias. Injecting carbon nanostructures in living cells. volume 2844, page 80 – 82, 2020

23 Anastasios Gotzias. Binding free energy calculations of bilayer graphenes using molecular dynamics. *Journal of Chemical Information and Modeling*, 61(3):1164 – 1171, 2021

24 Anastasios Gotzias, Andreas Sapalidis, and Evangelos Favvas. Hydrogen adsorption simulations in isomorphous borohydride and imidazolate frameworks: Evaluations using interpolation. *International Journal of Hydrogen Energy*, 46(37):19778 – 19787, 2021

25 Anastasios Gotzias, Elena Tocci, and Andreas Sapalidis. On the consistency of the exfoliation free energy of graphenes by molecular simulations. *International Journal of Molecular Sciences*, 22(15), 2021. All Open Access, Gold Open Access, Green Open Access

26 Anastasios Gotzias. Water to cyclohexane transfer free energy calculations for a carbon nanotube. *Carbon Trends*, 9, 2022. All Open Access, Gold Open Access

27 Chiara Muzzi, Anastasios Gotzias, Enrica Fontananova, and Elena Tocci. Stability of graphene oxide composite membranes in an aqueous environment from a molecular point of view. *Applied Sciences (Switzerland)*, 12(7), 2022. All Open Access, Gold Open Access

28 M. Pachoulis, A.A. Sapalidis, E.P. Kouvelos, A. Gotzias, G.Z. Kyzas, and E.P. Favvas. Study of cu2+ and dyes removal by sorption onto palygorskite in batch and continuous flow processes. *Desalination and Water Treatment*, 255:101 – 109, 2022

29 Anastasios Gotzias. Water to cyclohexane transfer free energy calculations for a carbon nanotube. *Carbon Trends*, 9, 2022. All Open Access, Gold Open Access

30 Anastasios Gotzias, Elena Tocci, and Andreas Sapalidis. Solvent-assisted graphene exfoliation from graphite using umbrella sampling simulations. *Langmuir*, 39(50):18437 – 18446, 2023

31 A. Gotzias and Y. G. Lazarou. Graphene exfoliation in binary nmp/water mixtures by molecular dynamics simulations. *ChemPlusChem*, 2024:e202300758

32 George V. Theodorakopoulos, Dionysios S. Karousos, Evangelos P. Favvas, and Anastasios Gotzias. Formation of polyimide membranes via non-solvent induced phase separation: Insight from molecular dynamics simulations. *ChemPlusChem*, 2024:e202300766

33 Fahmi Anwar, Anish Mathai Varghese, Suresh Kuppireddy, Anastasios Gotzias, Maryam Khaleel, Kean Wang, and Georgios N. Karanikolos. High-purity ethylene production from ethane/ethylene mixtures at ambient conditions by ethane-selective fluorine-doped activated carbon adsorbents. *ACS Applied Materials & Interfaces*, 17(5):8619–8633, 2025. PMID: 39862162

Papers submitted

34 A. Gotzias, Charitomeni Veziri, George Theodorakopoulos and George Romanos. Water-Induced CO2 Adsorption in ZIF-8: Insights from Experiments and Advanced Monte Carlo Simulations. Submitted to *Physical Chemistry Chemical Physics* (PCCP) in June 2025.

35 George V. Theodorakopoulos, Evangelos P. Kouvelos, Evangelos P. Favvas, and Anastasios D. Gotzias. Extending Ideal Adsorbed Solution Theory to Variable Temperatures: The T-IAST Approach. Submitted to *Microporous and Mesoporous Materials* in June 2025.

Papers in preparation (tentative titles)

36 A. Gotzias. Antibiotic Adsorption on Carbon Nanotubes: Insights by Steered Umbrella Sampling Simulations.

37 A. Gotzias. Simulate Before You Build. Molecular Dynamics Simulations for Green Membrane Development.

38 A. Gotzias. Thermodynamic Integration of Nanosheet Exfoliation in Organic Solvents.

39 A. Gotzias. Modeling Ternary Polymer–Solvent Equilibria Using Flory–Huggins Theory.

40 A. Gotzias. Molecular Water Permeation through Aquaporin Channels and Carbon Nanotubes.

Seminar and Conference Oral Presentations

2007: 3rd Pan-Hellenic Symposium of Porous Materials, PSPM-3 Thessaloniki, Greece

2007: 3rd Conference of Hellas Hydrogen Company, HELLASHY-3, Patras, Greece

2008: 4th Pan-Hellenic Symposium of Porous Materials, PSPM-4, Patras, Greece

2009: Workshop on solid storage of hydrogen, international perspectives, SSH-IP, Chania, Greece

2009: 7th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis, ISSHAC-7, Dolny, Poland

2011: Thermodynamics 2011, Athens, Greece

2011: 9th International symposium on the Characterisation of Porous Solids, COPS IX, Dresden, Germany

2011: 5th Pan-Hellenic Symposium of Porous Materials, PSPM-5, Chania, Greece

2012: 8th International Symposium Surface Heterogeneity Effects in Adsorption and Catalysis, ISSHAC-8, Krakow, Poland

2013: 6th Pan-Hellenic Symposium of Porous Materials, PSPM-6, Kavala, Greece

2014: 10th International Symposium on the Characterisation of Porous Solids, COPS-X, Granada, Spain

2014: CCP5 annual meeting, Condensed phase simulations, Telford, UK

2015: 7th International Conference on Porous Media & annual meeting of the International society of Porous Media, INTERPORE, Padova, Italy

2015: European Technical school on Hydrogen and Fuel Cells 2015, H2FC, Heraklion, Greece

2016: 7th Pan-Hellenic Symposium of Porous Materials, PSPM-7, Ioannina, Greece

2016: Hydrides as energy materials, HYDEM2016, Aarhus, Denmark

2017: 11th International Symposium on the Characterisation of Porous Solids, COPS-XI, Avignon, France

2018: Nanoporous Materials for green energy conversion and storage, 85th IUVSTA Workshop, Seggau, Austria

2019: 1st international gas adsorption summer school, i-gass, Spetses, Greece (invited lecturer)

2020: 12th International Symposium on the Characterisation of Porous Solids, COPS-XII, Bath, UK

2020: AINST2020 (AI in Natural Sciences and Technology - SETN2020 Workshop), Athens, Greece

2022: Euromembrane 2022, Sorrento, Naples, Italy

2023: MEDPore 23, Rethymnon, Crete, Greece

Involvement in Research Projects

FP7 GROWTH: *CERAMEM-LPG* Development of ceramic membranes for olefin recovery from liquefied petroleum gases (2010-2014)

FP7 NMP: *HYCONES* Hydrogen storage in carbon cones (2012-2017)

Greece Poland collaboration: Development and characterization of ordered porous materials for olefin - parafin gas separation. NCSR Demokritos - Institute of Chemical Engineering-Polish Academy of Sciences (2016-2017)

FP7 INFRASTRUCTURES-2011-1: *H2FC* Integrating European Infrastructure to support science and development of Hydrogen - and Fuel Cell Technologies towards European Strategy for Sustainable, Competitive and Secure Energy (2011-2015)

NSRF Greece-China collaboration: *IOLIPURE* aiming at the assessment of ionic liquid membranes and adsorbents for flue gas purification and carbon capture (2013-2015)

IDEA-ERANETMED2-72-357, Development of a solar powered, zero liquid discharge Integrated desalination membrane system to address the needs for water of the Mediterranean region (2017-2020) (WorkPackage Leader)

Research Grant Proposals

ESPA 2014-2020: "Support of new researchers " : BENCH - Screening crystallized nanomaterials for benzene cyclohexane separation. Academic Counsellor: MIS:5005985 (February 2017).

H.F.R.I. 2018: Action: 1^{st} call for H.F.R.I. Research Projects to support Faculty Members and Researchers. Title: Fast screening the olefin recovery performance of porous framework materials. Acronym: SCORE-MOFs. Proposal's Number: 3210, Scientific Area: SA2. Engineering Sciences & Technology. Grade 76.5 (January 2018)

ESPA 2014-2020: "Support of new researchers " : SCORE-MOFS - Fast screening the olefin recovery performance of porous framework materials, code number, 3210,grade 79.6 (February 2019).

H.F.R.I. 2020: Action: 2^{nd}Call for H.F.R.I. Research Projects to support Faculty Members and Researchers. Title: Carbon Nano Injections in living cells: Workflow design of molecular simulations, Acronym: CONNECT. Proposal s Number: 0358, Scientific Area: SA2. Engineering Sciences & Technology. Date of Submission: 31/05/2020.

ERC Consolidator Grant 2021 (HORIZON). Call reference: ERC-2021-COG. Title: Injecting Carbon Nanostructures in Living Cells: Workflow Design of Molecular Simulations, Acronym: INJECT. Proposal No: 101045546. Panel: LS6- Biotechnology and Biosystems Engineering. Date of Submission: 20/04/2021.

H.F.R.I. 2022 Sub-action 2. Funding Projects in Leading-Edge Sectors – RRFQ: Basic Research Financing (Horizontal support for all Sciences). Title: Removal of antibiotics from aqueous solutions using carbon adsorbents; From free energy simulations to experimental interpretation, Acronym: ADSORB. Proposal No: 015841. Date of submission: 10/10/2022.

3rd Call for H.F.R.I.'s Research Projects to Support Faculty Members & Researchers H.F.R.I. 2022. Title: Adsorptive Removal of Antibiotics from Wastewater by porous solids using Molecular Dynamics Simulations, Acronym: ADSORB. Proposal No: 26053. Date of submission: 15/01/2024.

Personal

Born on November 27, 1975.

Hellenic Nationality.

Married, 3 children.