Anastasios Gkotzias

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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:
Developing codes for post processing simulated isotherms relevant to the characterization of porous solids based on gas adsorption. Employing machine learning techniques for screening the performance of materials for gas storage and separation. Formulating and executing workflows committed to free energy simulations for liquid - solid and gas - solid interfaces. Reaching expertise in using different molecular dynamics and Monte Carlo software.

Research interests and skills

I formulate a sustainable computational workflow committed to free energy simulations. Practicing with well - defined force fields, I established a lower bound on the sampling necessary to simulate complex low dimensional materials like functionalized graphenes, metal oxides, hydrides, and metal organic framework nanosheets (MONs).

I study the biocompatibility of carbon interfaces. The workflow of free energy simulations is a precursor on an ongoing computational campaign modeling how the carbon nanoparticles may replicate the affinity and transport properties of proteins and how the carbon interface binds to the cholesterol supporters of living cells.

I simulate quantum sieving effects in nanosized confinements using the Grand canonical Monte Carlo (GCMC) method. I use the Feynmann - Hibbs potential to model hydrogen intermolecular interactions. The Feynmann - Hibbs potential includes the molecular masses of the interacting particles in the calculations. This is critical when simulating light mass adsorbates like hydrogen, because it provides a coarse description for quantum behaviour that can be computed inline. To date, there is no other available GCMC simulation package implementing the Feynmann - Hibbs potential.

I developed a tool building molecular models of carbon nanocones and nanohorns (nanotubes capped with sharp cones at one edge). Carbon cones can be formed with five different tip angles depending on the number (1-5) of pentagonal carbon rings near the tip. The pentagons give the apropriate surface curvature around the tip of the nanocones. The models of carbon nanocones may comprise up to 10,000 carbon atom coordinates (along with terminated hydrogen atoms at the boundaries). The output format is fully compatible with the GROMACS simulation modules.

I parameterize the oxygen content of carbon surfaces in molecular adsorption simulations. The oxygen content is regarded as an explicit source of surface heterogeneity. I use the parameterized simulations to assess information of the surface chemistry of oxidized graphites and graphene nanosheets based on gas adsorption experiments of carbon samples. The method has been proved more reliable and efficient than the relevant analysis methods embedded in different commercial instrumentation software.

Codes developed

Hycones software: Dedicated molecular simulation code for the prediction of H_2 sorption isotherms of single - angle carbon cones at different P-T conditions. The code incorporates Feynmann Hibbs quantum interactions and the path integral Monte Carlo definition making it capable to simulate light adsorbate particles. The module includes the only currently available routine that generates reliably multilayered carbon cones and disks of any size with a correct bonding topology. The software can simulate the competitive adsorption of simple gas mixtures. The code is being redesigned to exploit parallelism.

Auto_ Rubo routine: Module performing successive calibrations and tarings of the mass balance on a gravimetric analysis instrument. It is encoded in a user interface software (LabView), and runs in real time measurements. It performs a buoyancy correction for the sample inside the chamber. The boyancy changes due to the change of bulk pressure. The module estimates the equilibration time and predicts the adsorbed mass at the end of the measurement (equilibrium).

IAST solution: Solution algorithm estimating the competitive adsorption of adsorbate mixtures, regardless of the number of adsorbates. It uses analytical expressions with fitting parameters to describe the pure component isotherms.

Pore Size regularization: Method to calculate a distribution function from a desorption isotherm. The distribution describes the heterogeneous properties of a porous solid. The method is based on the

Tikhonov regularisation of discrete ill-posed problems and uses the truncated Singular Value Decomposition (TSVD) solver. The method can be applied to train machine learning models for screening the adsorption performance of porous materials.

Density splitter: A post process tool for GCMC adsorption simulations. It divides the cylindrical pore channels of a crystal into concentric regions of equal thickness δr and records the number of particles $N(r)$, located inside the regions $[r + \delta r]$. It returns averaged density distributions of the adsorbate.

Multiplot generator: Application that makes arrays of multiple panels of graphs and/or graph insets. The user specifies the arrangement of the panels, the number of plots in the graphs, the key legends and the axis details. The function is written in 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).

Programming languages and tools

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

Simulation Packages: GROMACS, MuSiC, iRaspa, 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.

Secretary at the scientific council of Physical Chemistry Institute (subsequently called 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* A. Sapalidis, Ed. Boca Raton: CRC Press, 2021

Refereed Journal Papers

3 K.A. Stoitsas, Gotzias, A., 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. cited By 25

4 Gotzias, A., 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. cited By 26

5 Gotzias, A., H. Heiberg-Andersen, M. Kainourgiakis, and T. Steriotis. A grand canonical monte carlo study of hydrogen adsorption in carbon nanohorns and nanocones at 77 k. *Carbon*, 49(8):2715–2724, 2011. cited By 18

6 Gotzias, A., E. Tylianakis, G. Froudakis, and T. Steriotis. Theoretical study of hydrogen adsorption in oxygen functionalized carbon slit pores. *Microporous and Mesoporous Materials*, 154:38–44, 2012. cited By 29

7 Gotzias, A. and T. 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. cited By 12

8 Gotzias, A., G. Charalambopoulou, A. Ampoumogli, I. Krkljus, M. Hirscher, and T. Steriotis. Experimental and theoretical study of d2/h2 quantum sieving in a carbon molecular sieve. *Adsorption*, 19(2-4):373–379, 2013. cited By 5

9 Gotzias, A., E. Tylianakis, G. Froudakis, and T. Steriotis. Effect of surface functionalities on gas adsorption in microporous carbons: A grand canonical monte carlo study. *Adsorption*, 19(2-4):745–756, 2013. cited By 15

10 I. Krkljus, T. Steriotis, G. Charalambopoulou, Gotzias, A., and M. Hirscher. H2/d2 adsorption and desorption studies on carbon molecular sieves with different pore structures. *Carbon*, 57:239–247, 2013. cited By 21

11 K.V. Kumar, G. Charalambopoulou, M. Kainourgiakis, Gotzias, A., A. Stubos, and T. 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. cited By 3

12 Gotzias, A., 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. cited By 13

13 Gotzias, A., G. Charalambopoulou, and T. 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. cited By 7

14 Gotzias, A. The effect of gme topology on multicomponent adsorption in zeolitic imidazolate frameworks. *Physical Chemistry Chemical Physics*, 19(1):871–877, 2017. cited By 8

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

16 Gotzias, A., E. Kouvelos, and A. Sapalidis. Computing the temperature dependence of adsorption selectivity in porous solids. *Surface and Coatings Technology*, 350:95–100, 2018. cited By 3

17 Gotzias, A. Calculating adsorption isotherms using lennard jones particle density distributions. *Journal of Physics Condensed Matter*, 31(43), 2019. cited By 2

18 G. Karataraki, A. Sapalidis, E. Tocci, and Gotzias, A. Molecular dynamics of water embedded carbon nanocones: Surface waves observation. *Computation*, 7(3), 2019. cited By 5

19 I.N. Floros, E.P. Kouvelos, G.I. Pilatos, E.P. Hadjigeorgiou, Gotzias, A.D., E.P. Favvas, and A.A. Sapalidis. Enhancement of flux performance in ptfe membranes for direct contact membrane distillation. *Polymers*, 12(2), 2020. cited By 10

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

21 A.G. Kontos, G.E. Romanos, C.M. Veziri, Gotzias, A., M.K. Arfanis, E. Kouvelos, V. Likodimos, G.N. Karanikolos, and P. Falaras. Correlating vibrational properties with temperature and pressure dependent co2 adsorption in zeolitic imidazolate frameworks. *Applied Surface Science*, 529, 2020. cited By 6

22 Gotzias, A. Injecting carbon nanostructures in living cells. In *CEUR Workshop Proceedings*, volume 2844, pages 80–82, 2020. cited By 0

23 Gotzias, A. Binding free energy calculations of bilayer graphenes using molecular dynamics. *Journal of Chemical Information and Modeling*, 61(3):1164–1171, 2021. cited By 1

24 Gotzias, A., A. Sapalidis, and E. Favvas. Hydrogen adsorption simulations in isomorphous borohydride and imidazolate frameworks: Evaluations using interpolation. *International Journal of Hydrogen Energy*, 46(37):19778–19787, 2021. cited By 1

25 Gotzias, A., E. Tocci, and A. Sapalidis. On the consistency of the exfoliation free energy of graphenes by molecular simulations. *International Journal of Molecular Sciences*, 22(15), 2021. cited By 0

Papers submitted

26 A. Gotzias. Umbrella Sampling Simulations of Carbon Nanoparticles Grossing Immiscible Solvents. December 2020. Submitted to *Molecules*.

Papers in preparation

27 A. Gotzias and E. Tocci and A. Sapalidis. Free energy calculations of Carbon Nanoparticles embedded in polar solvents.

28 A. Gotzias. Water Molecules Passing Through the Channels of Aquaporins and Carbon Nanotubes using Steered Molecular Dynamics.

Seminar and Conference 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

Involvement in Research Projects

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 Leading)

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

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)

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 (2006-2007)

FP6 NMP: *HYCONES* Hydrogen storage in carbon cones (2006-2009).

FP5 GROWTH: *CERAMEM-LPG* Development of ceramic membranes for olefin recovery from liquefied petroleum gases (2001-2005)

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: Carbons Nano Injectors 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.

Personal

Born on November 27, 1975.

Hellenic Nationality.

Married, 3 children.

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http://inn.demokritos.gr/en/prosopiko/a.gotzias/