Emmanuel N. **Koukaras**

Assistant Professor of Applied Quantum Chemistry

CONTACT – PERSONAL INFORMATION

Address:	Laboratory of Quantum and Computational Chemistry, School of Chemistry, Aristotle University of Thessaloniki (AUTH) University Campus, GR-54124, Thessaloniki, Greece
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ORCID:	0000-0002-5069-8334
ResearcherID:	F-7982-2011
Google Scholar ID:	5ipwQVcAAAAJ
Date of birth:	December 6, 1972
Place of birth:	Bronx, New York, U.S.A.
Family status:	Married, 2 children
Nationality:	Greek
Military obligations:	Fulfilled

EDUCATION

PhD University of Patras, Department of Physics **2006 – 2010**

Dissertation: Theoretical study of silicon-based nanoparticles and nanosystems.

MSc University of Patras, Department of Physics **2003 – 2006**

Field: Theoretical and Computational Physics

Thesis: Theoretical study of semiconductor atomic clusters. Silicon clusters with embedded transition metals.

BSc University of Patras, Department of Physics **1992 – 2003**

Field: Computational Molecular Physics

Thesis: Development of super cell applications in real space.

EXPERIENCE

Assistant Professor **2019 – present**

Aristotle University of Thessaloniki

Assistant professor of Applied Quantum Chemistry. Affiliated with the Laboratory of Quantum and Computational Chemistry of the Department of Chemistry.

Principle Investigator **2018 – present**

Foundation for Research and Technology (FORTH) /
Institute of Chemical Engineering Sciences (ICE-HT)

Principle investigator of the multi-disciplinary research project funded by the Hellenic Foundation for Research and Innovation (HFRI), in the framework of research grants to Support

Postdoctoral Researcher. The title of the project is «Designing pillared graphene nanomaterials with tuneable electronic properties and enhanced flexibility for electronic devices» (Grant agreement no.: 1536). Scientific Research Area *Natural Sciences*. Evaluation grade: 86.5. Rank: 16th place out of 24 funded.

Research Associate **2017 – 2019**

Hellenic Open University

Academic Associate of the School of Science and Technology of the Hellenic Open University. 2nd year Laboratory Thematic Module *Physics Laboratory I*. 4th year Laboratory Thematic Module *Physics Laboratory II*. Tutor–Student meetings. In person training of students on laboratory exercises. Creation of new didactic content.

Research Associate **2012 – 2018**

Foundation for Research and Technology (FORTH) /
Institute of Chemical Engineering Sciences (ICE-HT)

FORTH Graphene Center, and Composites and Nanostructured Materials Laboratory (CNM). Characterization of nanomaterials. Theoretical modeling of graphene. Theoretical study of graphene under mechanical loads. Mechanics and spectroscopy of graphene. Development of computer code for the study, via molecular dynamics, of graphene under mechanical loads. Study of the effects of load on the vibrational spectrum.

Research Associate **2011 – 2012**

Aristotle University of Thessaloniki

Department of Chemistry. Laboratory of Organic Technology. Theoretical study of novel nanocarriers for drug delivery.

Visiting Professor **2010 – 2011**

Higher Technological Educational Institute of Lamia

Department of Informatics and Computer Technology, *Basic electronics*, *Digital systems I*. Department of Electronics, *Low frequency electronics*.

Physics Laboratory Lecturing **2004 – 2006**

University of Patras

Department of Physics, Laboratories of *Mechanics*, *Electromagnetism*, *Optics*, *Waves*, *Nuclear Physics*, as well as *Computer Programming* (FORTRAN).

Scholarship | Basic Research Grant «K. Karatheodori 2003» **2003 – 2006**

University of Patras / Research Committee

Scholarship and Participation in the Basic Research Grant «K. Karatheodori 2003» (code: b.137) from the Research Committee of the University of Patras for the project entitled «First Principle (*ab initio*) theoretical study of nanomaterials of high scientific and technological importance».

Scholarship | Grant «Equipment Purchase» **2006 – 2008**

University of Patras

Scholarship and Participation in the Grant «Equipment Purchase» (code: 308) from the Research Committee of the University of Patras.

EXPERIENCE *PRO BONO*

Lecturer **2010 – 2011**

University of Patras

Department of Physics, Postgraduate course *Quantum Structure of Matter*. Assignment by Physics Department general assembly decision 2/25-10-10 G.S.E.S. (G.A.S.C.).

Assistant Lecturer **2007 – 2010**

University of Patras

Department of Physics. Lecturing, laboratory training, and tutoring sessions of the undergraduate course *Modern Physics* (Introduction to Quantum Physics) and *Contemporary Physics* (Nanotechnology).

Research Grant «Pythagoras I» **2004 – 2007**

University of Patras

Participation in the National Basic Research Grant «Pythagoras I» (code: b.365.030) for the project entitled « Design of Technologically Advanced Materials (Nanotechnology and Catalysis)».

Administrator of High-Performance Computing System **2003 – 2010**

University of Patras

Department of Physics. [First Phase] Technical Architecture and Design of the Molecular Engineering Group's Computer Cluster (BEOWULF named Moly). [Second Phase] Network & Systems Administration for the aforementioned cluster.

Hellenic Military **2000 – 2001**

Operator of Mobilization Section Data Processing | 32 Mobilization Unit | Serres
3rd Office, Military Training and Security | 535 Panzer Unit | Feres
Operator of Training Center Enlistment Procedure | 32 Mobilization Unit | Korinthos

System Administrator and IT Support **1993 – 1997**

University of Patras

System administrator and technical support (including hardware assembly and maintenance) at the Computer Center of the Department of Physics.
Administrative responsibilities on the following systems:

- Network based on Novell Netware 3.12
- Microsoft Networks with MS Windows NT 4.0 Server as Domain Controller
- Unix servers (Linux Slackware and assistant on HP-UX and IRIX)

PARTICIPATION IN RESEARCH PROGRAMS – AWARDS

GRAFEL | HFRI / GSRT | Principle Investigator **08 / 2018 – present**

Grant agreement no.: 1536

Title: Designing pillared graphene nanomaterials with tuneable electronic properties and enhanced flexibility for electronic devices.
Work Assigned: Principle Investigator, *Ab Initio* Computational Studies
Budget: € 449,990.11

ERC Advanced Research Grant | FP7-IDEAS-ERC **09 / 2015 – 05 / 2018**

Grant agreement no.: 321124, code: ΖΦΠ-13514-1

Title: Tailoring Graphene to Withstand Large Deformations.
Work Assigned: Theoretical modeling of graphene and graphene ribbons

ERC-10 | GSRT **06 / 2014 – 08 / 2015**

Grant agreement no.: MIS-374071, code: ΣΠΑ13491-1-1

Title: Deformation, Yield and Failure of Graphenes and Graphene based Nanocomposites.

Work Assigned: Characterization of nanomaterials

Graphene FET Flagship | FP7-ICT **03 / 2013 – 05 / 2013**

Grant agreement no. 604391, code: ΖΦΠ13516-1-1

Title: Graphene-Based Revolutions in ICT and Beyond.

Work Assigned: Theoretical modeling of graphene

Thales | ESF, NSRF **03 / 2013 – 02 / 2014**

Grant agreement no.: MIS-380389, code: ΣΠΑ13493-1-2

Title: Graphene and its nanocomposites: Production, properties and applications

Work Assigned: Computational study of chemically modified graphene with polymers and chromophore groups

SEB – Lodge of the Greek Industry **01 / 2013 – 02 / 2013**

Grant code: ΠΑΡ134668-1

Work Assigned: Mechanics and spectroscopy of graphene

Support Research Force of FORTH/EIXHMYTH | Region of Western Greece **2012 – 2013**

Grant agreement no: ΠΔΕ-312121, code: ΣΠΑ-13461-1

Title: Mechanics and spectroscopy of graphene

Work Assigned: Theoretical study of graphene under mechanical loads

EYDE-ETAK | GSRT | MELLRA **2011 – 2012**

Grant code: 84917

Title: Development of novel nanocarriers of Ixabepilone and examination of potential for applications in the treatment of breast cancer. Work Package (ΕΕ1) / Preliminary study, synthesis and characterization of polymers

Work Assigned: Π1.5 Copolymers Poly (alkylene dicarboxylates)

Work Assigned: Π1.9 Attachment of folic acid at edges of copolymers Polly (alkylene dicarboxylates)/PEG via ester or amidic bond

Work Assigned: Π1.10 Study of physicochemical characteristics of as produced polymers by suitable analysis techniques

Award **2008**

Young Scientist Excellence Award

Context: International Conference of Computational Methods in Sciences and Engineering 2008

Presentation/Paper Title: Multidecker stacking and cluster fusion of silicon–carbon clusters

Pythagoras I | ESF, EPEAEK II **2004 – 2007**

Grant agreement no: b.365.030

Title: Design of technologically advanced materials (Nanotechnology and Catalysis)

Work Assigned: First principle computations on surface oxygen bonding of anatase (*pro bono*, member or Project Research Group, assistance in computational aspects)

K. Karatheodori **2003 – 2006**

Grant agreement no: b.137

Title: First Principle (*ab initio*) theoretical study of nanomaterials of high scientific and technological importance

Work Assumed: First principle computations on transition metal doped silicon nanoclusters

PRESENTATIONS

CMD26 | Invited **2016**

Examining the response of graphene and other 2D crystals under mechanical loads

INVITED Talk at the International Conference of the Condensed Matter Division of the European Physical Society (EPS) (CMD26), 4 – 9 September 2016, Groningen, The Netherlands.

Nanotheo 2013 **2013**

Density Functional Theory, The Route to Chemical Accuracy

Theoretical and Computational Nanophysics and Chemistry Workshop of the Nanomaterials Theoretical Design Intra-University Network (Nanotheo 2013), 21 May 2013, University of Patras, Patras, Greece.

ICCMSE 2010 **2010**

All Electron *Ab Initio* Calculations for the Interaction of Glycine and Tyrosine with Metal–Organic–Frameworks (MOFs)

International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2010), 03 – 08 October 2010, Psalidi, Kos, Greece.

ICCMSE 2008 (Awarded) **2008**

Multidecker Stacking and Cluster Fusion of Silicon–Carbon Clusters

International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2008), 25 – 30 September 2008, Hersonissos, Crete, Greece, Greece.

Micro & Nano 2007 **2007**

High-stability finite-length silicon nanowires: A real space theoretical study

Third International Conference Micro & Nano (Micro & Nano 2007), 18 – 21 November 2007, NCSR Demokritos, Athens, Greece.

ICCMSE 2006 **2006**

Ab initio study of optical and electronic properties of silicon Nanowires

International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2006), 27 October – 1 November 2006, Chania, Crete, Greece.

ICCMSE 2005 **2005**

Structural and Electronic Properties of the $Ni@Si_{12}$ nanocluster

International Conference of Computational Methods in Sciences and Engineering (ICCMSE 2005), 21 – 26 October 2005, Loutraki, Korinthos, Greece.

INTERNATIONAL AND DOMESTIC PROFESSIONAL SERVICES

Reviewer of International Journals and Funding Agencies

American Chemical Society Petroleum Research Fund
ACS Journal of the American Chemical Society (JACS)
Springer Graphene Technology
ACS Industrial & Engineering Chemistry Research
Elsevier International Journal of Hydrogen Energy
RSC Physical Chemistry Chemical Physics (PCCP)

Elsevier Materials Science in Semiconductor Processing
Advanced Composites Letters (prior to SAGE)
RSC Advances
Materials Today
NPG Scientific Reports
T&F Molecular Simulation
IOS Journal of Computational Methods in Sciences and Engineering
Physics and Chemistry of Solids
American Chemical Society Petroleum Research Fund

Committees

Member, Local Organizing Committee

Workshop on Graphene: Second Graphene Summer School, FORTH Graphene Center, Patras, Greece, July 14–18, 2014

Volunteer, Scientific Support Desk

Industrial Technologies 2014 Conference, Athens International Conference Centre Megaron, Greece, April 9–11, 2014

Industrial Technologies 2014 is a Greek Presidency 2014 event under the auspices of the General Secretariat of Research & Technology (GSRT).

Member, Scientific Program Committee

First Workshop on Theoretical and Computational Nanophysics and Chemistry, Patras, Greece, May 31, 2013

AVOCATIONAL PRODUCTIVITY | SKILLS

Programming (Primary: C/C++, Fortran, Assembly x86 and 8085)

GRchiral

A program for the design of chiral orthogonal unit cell and chiral orthogonal extended computational cells, with adjustable dimensions and rotational angles with respect to zig-zag direction of graphene. Additional capabilities include edge polishing, coordinate transformation, and supports file formats of well-known computational packages (xyz, lammps data file, gaussian job files). The source code is written in Fortran 90 and is portable on compilers (GNU, Intel) and operating systems (Windows, Linux). The main application of the program was to assist in the development of the programs PHDOS and PHDISP. Development was initiated within a project for the study of the mechanical properties of graphene under mechanical loads, at FORTH/ICE-HT.

PHDISP

A program for computing phonon dispersion curves by processing data from molecular dynamics simulations. The development was done in a generic manner to import formatted data from well-known commercial molecular dynamics packages. The implemented method is within the Green–Kubo formalism and is independent of the underlying level of theory on which the molecular dynamics simulations are performed (*ab initio*, DFT, CPMD, TBMD, MM/MD). The source code is written in C/C++ and is portable on compilers (Visual C, GNU, Intel) and operating systems (Windows, Linux). Development was initiated within a project for the study of the mechanical properties of graphene under mechanical loads, at FORTH/ICE-HT.

PHDOS

A program for computing phonon density of state by processing data from molecular dynamics simulations. The source code is written in C/C++ and is portable on compilers (Visual

C, GNU, Intel) and operating systems (Windows, Linux). Development was initiated within a project for the study of the mechanical properties of graphene under mechanical loads, at FORTH/ICE-HT.

PCHAIN

A program that simulates a chain of particles under the influence of a nearest neighbor potential. The method of integration of equations of motion is chosen amongst 6 different implemented algorithms. The source code is written in Fortran 90 and is portable on compilers (GNU, Intel) and operating systems (Windows, Linux). The main application of the program was to assist in the development of the programs PHDOS and PHDISP. Development was initiated within a project for the study of the mechanical properties of graphene under mechanical loads, at FORTH/ICE-HT.

SCFENGINE

A program for electronic structure calculations from first principles. The program numerically solves the Schrödinger equation using the Hartree–Fock method. It includes all of the well-known Gaussian type basis sets from modern literature. Design and implementation of highly optimized linear algebra algorithms which make use of the extended instruction set SSE2 (SIMD) and include directives to respect the cacheline. The source code is written in C/C++ and is portable on compilers (Visual C, GNU, Intel, and PGI) and operating systems (Windows, Linux and HP-UX). Development was from scratch and took place in context of my Ph.D.

COOPDOS

A program for processing results from electronic structure of matter calculations. It performs Crystal Orbital Overlap Population (COOP) analysis and produces the corresponding diagrams. Executable on Windows and Linux.

MOLVIEW

A program for visualization of three-dimensional molecular structures. All vector transformation and visualization routines were written from scratch with no usage of 3D acceleration hardware. Execution limited on DOS in protected mode. Compiled using Watcom 10.5 C/C++ with DOS4GW (PMode DOS Extender). For more information visit: http://moleng.physics.upatras.gr/personnel/Koukaras/molview.html

LASCC

A Win32 console utility for preprocessing data and creating super cells prior prepared for electronic structure calculations. The source code is written in C/C++ and is portable on compilers (Visual C, GNU, Intel) and operating systems (Windows, Linux). Compiled using Microsoft Visual Studio 6.0. Development took place in context of my bachelor's degree.

Microelectronics

i8085 8-bit prototype

Design and prototypical implementation of a fully functional 8-bit computer based on the Intel 8085 processor and interconnected to a graphical LCD screen via a custom data-bus interface. The system is complemented with a BIOS coded from scratch in assembly 8085 that includes graphics display routines. For images and more information visit: http://moleng.physics.upatras.gr/personnel/Koukaras/GMK.html

PLDasm

Programming PLDs in PLDasm using ALTERA's PLDshell Plus 5.

ARM 7TDMI

Coding embedded systems based on the ARM 7TDMI processor using the ARM Software Development Toolkit 2.50. Final code tested only on emulators, not on the actual systems.

RESEARCH COLLABORATIONS

National (Active | Recent)

Prof. Constantine Galiotis, Department of Chemical Engineering, University of Patras
Prof. Michael M. Sigalas, Department of Materials Sciences, University of Patras
Prof. Costantinos Papaggelis, Department of Physics, Aristotle University of Thessaloniki
Assist. Prof. George Kalosakas, Department of Materials Sciences, University of Patras
Prof. Demetrios Bikiaris, Department of Chemistry, Aristotle University of Thessaloniki
Prof. George Froudakis, Department of Chemistry, University of Crete
Assist. Prof. Panaghiotis Angaridis, Department of Chemistry, Aristotle University of Thessaloniki
Prof. Emeritus Aristides D. Zdetsis, Department of Physics, University of Patras

International (Active | Recent)

Prof. Ganesh Datt Sharma, LNM Institute of Information Technology, Jaipur, India
Prof. Mukhamed L. Keshtov, Institute of Organoelement Compounds of the Russian Academy of Sciences, Moscow, Russian Federation
Dr. Panagiotis Karamanis, Université de Pau et des Pays de l'Adour, France

PUBLICATIONS

A. International Scientific Indexed (ISI) Journals

74. Porous carbon nanotube networks and pillared graphene materials exhibiting high SF_6 adsorption uptake and separation selectivity of SF_6/N_2 fluid mixtures: A comparative molecular simulation study,
Ioannis Skarmoutsos, Emmanuel N. Koukaras, Costas Galiotis, George E. Froudakis, Emmanuel Klontzas,
Microporous and Mesoporous Materials JUST ACCEPTED XXX, XXX–220 (2020)
DOI: JUST ACCEPTED

73. Enhancement of photovoltaic efficiency through fine adjustment of indacene-based non-fullerene acceptor by minimal chlorination for polymer solar cells,
Mukhamed. L. Keshtov, Sergei. A. Kuklin, Chuandong Dou, Emmanuel N. Koukaras, Rahul Singhal, Prateek Malhotra and Ganesh D. Sharma,
Nano Select JUST ACCEPTED XXX, XXX–220 (2020)
DOI: 10.1002/nano.202000027

72. New Donor-Acceptor polymers with a wide absorption range for photovoltaic applications,
M. L. Keshtov, S. A. Kuklin, I. O. Konstantinov, I. E. Ostapov, Zh. Xie, Emmanuel N. Koukaras, Rakesh Suthar and Ganesh D. Sharma,
Solar Energy 205, 211–220 (2020)
DOI: 10.1016/j.solener.2020.05.059

71. Effect of poly(vinyl alcohol) on nanoencapsulation of budesonide in chitosan nanoparticles via ionic gelation and its improved bioavailability for inhaled administration,
Georgia Michailidou, Nina Maria Ainali, Eleftheria Xanthopoulou, Stavroula Nanaki, Margaritis Kostoglou, Emmanuel N. Koukaras, Dimitrios N. Bikiaris,
MDPI Polymers 12(5), 1101 (2020)

DOI: 10.3390/polym12051101

70. Thermomechanical Response of Supported Hexagonal Boron Nitride Sheets of Various Thicknesses,
Lambros Seremetis, Emmanuel N. Koukaras, Sotiria Alexandri, Antonis Michail, George Kalosakas, John Parthenios, Costas Galiotis, Sotirios Tsirkas, Spyridon Grammatikopoulos, and Konstantinos Papagelis,
ACS Journal of Physical Chemistry Part C 124, 12134–12143 (2020)
DOI: 10.1021/acs.jpcc.0c01029

69. Cardanol and Guaiacol sourced Solution-Processable Green Small Molecules based Organic Solar Cells,
Barla Rajkumar, Lubna Khanam, Emmanuel N. Koukaras, Ganesh Sharma, Samarendra Singh, Bimlesh Lochab,
ACS Sustainable Chemistry & Engineering 8, 5891–5902 (2020)
DOI: 10.1021/acssuschemeng.9b07600

68. Tunable macroscale structural superlubricity in two-layer graphene via strain engineering,
Charalampos Androulidakis, Emmanuel N. Koukaras, George Paterakis, George Trakakis & Costas Galiotis,
NPG Nature Communications 11, 1595 (2020), **OPEN ACCESS**
DOI: 10.1038/s41467-020-15446-y

67. Synthesis and Photovoltaic Properties of New Conjugated D-A Polymers Based on the Same Fluoro-Benzothiadiazole Acceptor Unit and Different Donor Units,
Mukhaned L Keshtov, Serge. A. Kuklin, Ionv. O. Konstantinov, Alexei R. Khokhlov, Zhiyuan Xie, Chuandong Dou, Emmanuel N. Koukaras, Rakesh Suthar, Ganesh D. Sharma,
Wiley ChemistrySelect 5, 853 (2020)
DOI: 10.1002/slct.201904353

66. Stress-transfer from polymer substrates to monolayer and few-layer graphenes,
Ch. Androulidakis, D. Sourlantzis, E. N. Koukaras, A. C. Manikas, and C. Galiotis
RSC-Nanoscale Advances 1, 4972–4980 (2019)
DOI: 10.1039/C9NA00323A

65. Absorption spectrum of magnesium and aluminum hydride nanoparticles,
Alexandros Chronis, Michael M. Sigalas, and Emmanuel N. Koukaras
Elsevier Materials Chemistry and Physics 228, 244–253 (2019)
DOI: 10.1016/j.matchemphys.2019.02.081

64. Sculpturing Graphene Wrinkle Patterns into Compliant Substrates,
Krishna Sampathkumar, Charalampos Androulidakis, Emmanuel N. Koukaras, Jaroslava Rahova, Karolina Drogowska, Martin Kalbac, Aliaksei Vetushka, Antonin Fejfar, Costas Galiotis and Otakar Frank
Elsevier Carbon 146, 772–778 (2019)
DOI: 10.1016/j.carbon.2019.02.041

63. *Ab initio* study of medium sized boron doped silicon clusters Si_nB_m, n=11–13, m=1–3,
E. N. Koukaras
RSC Physical Chemistry Chemical Physics (PCCP) 20, 18556 (2018)

DOI: 10.1039/C8CP02771D

62. Strained hexagonal boron nitride: phonon shift and Grüneisen parameter,
Ch. Androulidakis, E. N. Koukaras, M. Poss, K. Papagelis, C. Galiotis, S. Tawfick
APS Physical Review B, Rapid Communication 97, 241414(R) (2018)
DOI: 10.1103/PhysRevB.97.241414

61. Non-Eulerian behavior of graphitic materials under compression,
Ch. Androulidakis, E. N. Koukaras, M. Hadjinicolaou, C. Galiotis
Elsevier Carbon 138, 227–233 (2018), **OPEN ACCESS**
DOI: 10.1016/j.carbon.2018.06.011

60. BODIPY–diketopyrrolopyrrole-porphyrin conjugate Small Molecules for Use in Bulk Heterojunction Solar Cells,
Léo Bucher, Nicolas Desbois, Emmanuel. N. Koukaras, Charles H. Devillers, Subhayan Biswas, Ganesh D. Sharma, and Claude P. Gros
RSC Journal of Materials Chemistry A 6, 8449 (2018)
DOI: 10.1039/c8ta01291a

59. Synthesis and photovoltaic properties of new D-A copolymers based on 5,6-bis(2-ethylhexyl)naphtha[2,1-b:3,4-b']dithiophene-2,9-diyl] donor and fluorine substituted 6,7-bis(9,9-didodecyl-9H-fluoren-2-yl)[1,2,5]thiadiazolo[3,4-g]quinoxaline acceptor units,
M. L. Keshtov, I. O. Konstantinov, S. A.Kuklin, A. R. Khokhlov, N. V. Nekrasova, Zhi-yuan Xie, E. N. Koukaras and Ganesh D. Sharma
Wiley Journal of Polymer Science, Part A: Polymer Chemistry 56, 1297–1307 (2018)
DOI: 10.1002/pola.29011

58. Dithienosilole–phenylquinoxaline-Based copolymers with D–A–D–A and D–A Structures for Polymer Solar cells,
M. L. Keshtov, A. R. Khokhlov, S. A. Kuklin, A. Yu. Nikolaev, E. N. Koukaras, and Ganesh D. Sharma
Wiley Journal of Polymer Science A: Polymer Chemistry 56, 376–386 (2018)
DOI: 10.1002/pola.28904

57. Wrinkling formation in simply-supported graphenes under tension and compression loadings,
Ch. Androulidakis, E. N. Koukaras, M. G. Pastore, M. Hadjinicolaou, and C. Galiotis
RSC Nanoscale 9, 18180–18188 (2017)
DOI: 10.1039/C7NR06463B

56. Wrinkled few-layer graphene as highly efficient load bearer,
Charalampos Androulidakis, Emmanuel N. Koukaras, Jaroslava Rahova, Krishna Sampathkumar, John Parthenios, Konstantinos Papagelis, Otakar Frank, and Costas Galiotis
ACS Advanced Materials & Interfaces 9, 26593–26601 (2017)
DOI: 10.1021/acsami.7b07547

55. Polymer Solar Cells Based Low Bandgap A1–D–A2–D Terpolymer Based on Fluorinated Thiadiazoloquinoxaline and Benzothiadiazole Acceptors with Energy Loss Less Than 0.5 eV,
M. L. Keshtov, D.Y. Godovskiy, S.A. Kuklin, A.R. Khokhlov, S.A. Osipov, N. A. Radychev, I.O. Konstantinov, F.C. Chen, E. N. Koukaras, and Ganesh D. Sharma

Elsevier Organic Electronics 46, 192–202 (2017)
DOI: 10.1016/j.orgel.2017.04.015

54. Computational study of the excitation energies of CdSe nanoparticles with defects,
Fotios I. Michos, Michail M. Sigalas, and Emmanuel N. Koukaras
IEEE Journal of Selected Topics in Quantum Electronics 23, 4800305 (2017)
DOI: 10.1109/JSTQE.2017.2665643

53. New D–A1–D–A2-type regular terpolymers containing benzothiadiazole and benzotrithiophene acceptor units for photovoltaic application,
Mukhamed L. Keshtova, Alexei R. Khokhlov, Serge A. Kuklin, Fang-Chung Chen, Emmanuel N. Koukaras and Ganesh D. Sharma
ACS Applied Materials & Interfaces 8, 32998 (2016)
DOI: 10.1021/acsami.6b08802

52. Synthesis and photophysical properties of semiconductor molecules D1–A–D2–A–D1-type structure based on derivatives of quinoxaline and dithienosilole for organics solar cells,
M. L. Keshtova, D. Yu. Godovsky, S. A. Kuklin, A. Nicolaev, J. Lee, J. Kim, B. Lim, H, K. Lee, E. N. Koukaras, Ganesh D. Sharma
Elsevier Organic Electronics 39, 361–370 (2016)
DOI: 10.1016/j.orgel.2016.10.010

51. Systematic spatial and stoichiometric screening towards understanding the surface of ultrasmall oxygenated silicon nanocrystal,
Shanawer Niaz, Aristides D. Zdetsis, Emmanuel N. Koukaras, Oğuz Gülseren, Imran Sadiq,
Elsevier Applied Surface Science 387, 771–778 (2016)
DOI: 10.1016/j.apsusc.2016.06.197

50. Design of diketopyrrolopyrrole chromophores applicable as sensitizers in dye-sensitized photovoltaic windows for green houses,
Naresh Duvva, Dimitris Raptis, Challuri Vijay Kumar, Emmanuel N. Koukaras, Lingamallu Giribabu, Panagiotis Lianos,
Elsevier Dyes and Pigments 134, 472–479 (2016)
DOI: 10.1016/j.dyepig.2016.07.046

49. Synthesis and photophysical properties of regioregular low bandgap copolymers with controlled 5-fluorobenzotriazole orientation for photovoltaic application,
M. L. Keshtov, A. R. Khokhlov, S. A. Kuklin, I. E. Ostapov, A. Yu. Nikolaev, I. O. Konstantinov, Abhishek Sharma, E. N. Koukaras and Ganesh D. Sharma,
RSC Polymer Chemistry 7, 5849–5861 (2016)
DOI: 10.1039/c6py01173j

48. New ultra low bandgap thiadiazolequinoxaline-based D–A copolymers for photovoltaic applications,
M. L. Keshtov, S. A. Kuklin, I. O. Konstantinov, I. E. Ostapov, M. A. Topchiy, A. R. Khokhlov, E. N. Koukaras, G. D. Sharma,
Elsevier Organic Electronics 37, 411–420 (2016)
DOI: 10.1016/j.orgel.2016.07.016

47. Synthesis of new D–A1–D–A2 type low bandgap terpolymers based on different thiadiazoloquinoxaline acceptor units for efficient polymer solar cells,
M. L. Keshtov, S. A. Kuklin, N. A. Radychev, I. E. Ostapov, A. Y. Nikolaev, I. O. Konstantinov, M. M. Krayushkin, E. N. Koukaras, A. Sharma, G. D. Sharma,
RSC Advances 6, 71232–71244 (2016)
DOI: 10.1039/c6ra14537j

46. Design, synthesis and photophysical properties of D1–A–D2–A–D1-type small molecules based on fluorobenzotriazole acceptor and dithienosilole core donor for solution processed organic solar cells,
M. L. Keshtov, D. Yu Godovsky, S. A. Kuklin, J. Lee, J. Kim, B. Lim, H. K. Lee, S. Biswas, E. N. Koukaras, G. D. Sharma,
Elsevier Dyes and Pigments 132, 387–397 (2016)
DOI: 10.1016/j.dyepig.2016.05.022

45. Synthesis of alternating D–A1–D–A2 terpolymers comprising two electron-deficient moieties, quinoxaline and benzothiadiazole units for photovoltaic applications,
M. L. Keshtov, A. R. Khokhlov, S. A. Kuklin, F. C. Chen, A. Y. Nikolaev, E. N. Koukaras, and G. D. Sharma,
RSC Polymer Chemistry 7, 4025–4035 (2016)
DOI: 10.1039/c6py00652c

44. Long-lived discrete breathers in free-standing graphene,
Alberto Fraile, Emmanuel N. Koukaras, Konstantinos Papagelis, Nikos Lazarides, G.P. Tsironis,
Elsevier Chaos, Solitons and Fractals 87, 262–267 (2016)
DOI: 10.1016/j.chaos.2016.04.015

43. Compression behavior of simply-supported and fully embedded monolayer graphene: theory and experiment,
Emmanuel N. Koukaras, Charis Androulidakis, Konstantinos Papagelis, George Anagnostopoulos, and Costas Galiotis,
Elsevier Extreme Mechanics Letters 8, 191–200 (2016)
DOI: 10.1016/j.eml.2016.03.016

42. Fully Hydrogenated Beryllium Nanoclusters,
Emmanuel N. Koukaras, Aris P. Sgouros, and Michael M. Sigalas,
ACS Journal of the American Chemical Society (JACS) 138, 3218–3227 (2016)
DOI: 10.1021/jacs.6b00135

41. New low band gap near-IR conjugated D–A copolymers for BHJ polymers solar cell applications,
Mukhamed Lostambievich Keshtov, S. A. Kuklin,Nikolay Radychev, A. Y. Nikolaev, I. E. Ostapov, M. M. Krayushkin, I. O. Konstantinov, Emmanuel N. Koukaras, Abhishek Sharma, and Ganesh D. Sharma,
RSC Physical Chemistry Chemical Physics (PCCP) 18, 8389–8400 (2016)
DOI: 10.1039/C5CP07705B

40. Design and synthesis of new ultra-low band gap thiadiazoloquinoxaline-based polymers for near infrared organic photovoltaic application,

M. L. Keshtov, S. A. Kuklin, N. A. Radychev, A. Yu. Nikolaev, E. N. Koukaras, Abhishek Sharma and G. D. Sharma,
RSC Advances 6, 14893 (2016)
DOI: 10.1039/c5ra24364e

39. Graphene flakes under controlled biaxial deformation,
Charalampos Androulidakis, Emmanuel N. Koukaras, John Parthenios, George Kalosakas, Konstantinos Papagelis, and Costas Galiotis,
NPG Scientific Reports 5, 18219 (2015), **OPEN ACCESS**
DOI: 10.1038/srep18219

38. Donor–acceptor–acceptor–donor small molecules for solution processed bulk heterojunction solar cells,
P. Gautam, R. Misra, E. N. Koukaras, Abhishek Sharma, G.D. Sharma,
Elsevier Organic Electronics 25, 72 (2015)
DOI: 10.1016/j.orgel.2015.09.006

37. Chitosan derivatives as effective nanocarriers for ocular release of timolol drug,
Panoraia I. Siafaka, Alexandra Titopoulou, Emmanuel N. Koukaras, Margaritis Kostoglou, Efthimios Koutris, Evangelos Karavas, Dimitrios N. Bikiaris,
Elsevier International Journal of Pharmaceutics 495, 249 (2015)
DOI: 10.1016/j.ijpharm.2015.08.100

36. Graphene as a hexagonal 2-lattice: evaluation of the in-plane material constants for the linear theory. A multiscale approach,
D. Sfyris, E. N. Koukaras, N. Pugno, C. Galiotis,
AIP Journal of Applied Physics 118, 075301 (2015)
DOI: 10.1063/1.4928464

35. New Alternating D–A1–D–A2 Copolymer Containing Two Electron-deficient Moieties Based on Benzothiadiazole and 9-(2-octyldodecyl)-8H-pyrrolo[3,4-b]bisthieno[2,3-f:3',2'-h]quinoxaline-8,10 (9H)-dione for Efficient Polymer Solar Cells,
M. L. Keshtov, S. A. Kuklin, D. Yu. Godovsky, A. R. Khokhlov, R. Kurchania, F. C. Chen, Emmanuel N. Koukaras and G. D. Sharma,
Wiley Journal of Polymer Science A: Polymer Chemistry 54, 155–168 (2016)
DOI: 10.1002/pola.27786

34. Phonon properties of graphene derived from molecular dynamics simulations,
Emmanuel N. Koukaras, George Kalosakas, Costas Galiotis, and Konstantinos Papagelis,
NPG Scientific Reports 5, 12923 (2015), **OPEN ACCESS**
DOI: 10.1038/srep12923

33. Efficient solution processed D1–A–D2–A–D1 small molecules bulk heterojunction solar cells based on alkoxy triphenylamine and benzo[1,2-b:4,5-b0]thiophene units,
Challuri Vijay Kumar, Lydia Cabau, Emmanuel N. Koukaras, Ganesh D. Sharma, Emilio Palomares,
Elsevier Organic Electronics 26, 36–47 (2015)
DOI: 10.1016/j.orgel.2015.07.014

32. A–π–D–π–A based porphyrin for solution processed small molecule bulk heterojunction solar cells,

Challuri Vijay Kumar, Lydia Cabau, Emmanuel N. Koukaras, Abhishek Sharma, Ganesh D. Sharma and Emilio Palomares,
RSC Journal of Materials Chemistry A 3, 16287 (2015)
DOI: 10.1039/c5ta03463a

31. Suspended monolayer graphene under true uniaxial deformation,
Ioannis Polyzos, Massimiliano Bianchi, Laura Rizzi, Emmanuel N. Koukaras, John Parthenios, Konstantinos Papagelis, Roman Sordan and Costas Galiotis,
RSC Nanoscale 7, 13033, (2015)
DOI: 10.1039/c5nr03072b

30. Study of an indoline–phenothiazine based organic dye for Dye-Sensitized Solar Cells. Theoretical calculations and experimental data,
Challuri Vijay Kumar, Dimitrios Raptis, Emmanuel N. Koukaras, Lamprini Sygellou, Panagiotis Lianos,
Elsevier Organic Electronic 25, 66–73 (2015)
DOI: 10.1016/j.orgel.2015.06.009

29. Graphene Mechanics: Current Status and Perspectives,
Costas Galiotis, Otakar Frank, Emmanuel N. Koukaras, Dimitris Sfyris,
AR Annual Review of Chemical and Biomolecular Engineering 6, 121–140 (2015)
DOI: 10.1146/annurev-chembioeng-061114-123216

28. Characterization of metal-free D-$(\pi\text{-}A)_2$ organic dye and its application as cosensitizer along with N719 dye for efficient dye-sensitized solar cells,
M. Singh, R. Kurchania, A. Pockett, R. J. Ball, E. N. Koukaras, P. J. Cameron and G. D. Sharma,
Springer Indian Journal of Physics 89, 1041–1050 (2015)
DOI: 10.1007/s12648-015-0681-0

27. Efficient bulk heterojunction solar cells based on solution processed small molecules based on same benzo[1,2-b:4, 5-b']thiophene unit as core donor and different terminal units,
Vijay Kumar, Lydia Cabau, Emmanuel N. Koukaras, S. A. Siddiqui, Ganesh D. Sharma and Emilio Palomares,
RSC Nanoscale 7, 7692 (2015)
DOI: 10.1039/C5NR01037C

26. Stress transfer mechanisms at the sub-micron level for graphene/ polymer systems,
George Anagnostopoulos, Charalampos Androulidakis, Emmanuel N. Koukaras, Georgia Tsoukleri, Ioannis Polyzos, John Parthenios, Konstantinos Papagelis , and Costas Galiotis,
ACS Applied Materials & Interfaces 7, 4216–4223 (2015), **OPEN ACCESS**
DOI: 10.1021/am508482n

25. Solution processed organic solar cells based on A–π–D–π–A Small Molecule with benzo[1,2-b:4,5-b']dithiophene donor unit and ethylrhodanine acceptor unit having 6 % light to energy conversion efficiency,
Challuri Vijay Kumar, Lydia Cabau, E. N. Koukaras, Aurelien Viterisi, G. D. Sharma and Emilio Palomares,
RSC Journal of Materials Chemistry A 3, 4892–4902 (2015)

DOI: 10.1039/C4TA05807K

24. Alternative use of cross-linked polyallylamine (known as Sevelamer pharmaceutical compound) as biosorbent,
George Z. Kyzas, Panoraia I. Siafaka, Dimitrios N. Bikiaris, Emmanuel N. Koukaras, George E. Froudakis,
Elsevier Journal of Colloid and Interface Science 442, 49–59 (2015)
DOI: 10.1016/j.jcis.2014.11.036

23. Synthesis, Optical and Electrochemical Properties of A–π–D–π–A Porphyrin and its Application as Electron Donor in Efficient Solution Processed Bulk Heterojunction Solar Cells,
Challuri Vijay Kumar, Lydia Cabau, E. N. Koukaras, Emilio J. Palomares and G. D. Sharma,
RSC Nanoscale 7, 179–189 (2015)
DOI: 10.1039/C4NR05565A

22. Donor-π-acceptor, triazine-linked porphyrin dyads as sensitizers for dye-sensitized solar cells,
Ganesh D. Sharma, Galateia E. Zervaki, Kalliopi Ladomenou, Emmanuel N. Koukaras, Panagiotis P. Angaridis, and Athanassios G. Coutsolelos,
WS Journal of Porphyrins and Phthalocyanines 19, 175–191 (2015)
DOI: 10.1142/S108842461450117X

21. Synthesis, optical and electrochemical properties new donor–acceptor (D–A) copolymers based on benzo[1,2-b:3,4-b':6,5-b"] trithiophene donor and different acceptor units: Application as donor for photovoltaic devices,
M. L. Keshtov, Y. Geng, S. A. Kuklin, A. R. Khokhlov, E. N. Koukaras, G. D. Sharma,
Elsevier Organic Electronics 17, 167–177 (2014)
DOI: 10.1016/j.orgel.2014.11.011

20. Synthesis and Photovoltaic Properties of New Donor–Acceptor (D–A) Copolymers Based on Benzo[1,2-b:3,4-b':6,5-b'']trithiophene donor and different acceptor units (P1 and P2),
G. D. Sharma, Mukhamed Lostambievich Keshtov, Y. Deng, Zhiyuan Xie, Yanhou Geng, E. N. Koukaras, A. R. Khokhlov, S. A. Kuklin, and V. S. Kochurov,
RSC Advances 4, 53531–53542 (2014)
DOI: 10.1039/C4RA05680A

19. *Ab initio* theoretical investigation of beryllium and beryllium hydride nanoparticles and nanocrystals with implications for the corresponding infinite systems,
Aristides D. Zdetsis, Michael M. Sigalas, Emmanuel N. Koukaras,
RSC Physical Chemistry Chemical Physics (PCCP) 16, 14172–14182 (2014)
DOI: 10.1039/C4CP01587H

18. Failure Processes in Embedded Monolayer Graphene under Axial Compression,
Charalampos Androulidakis, Emmanuel N. Koukaras, Otakar Frank, Georgia Tsoukleri, Dimitris Sfyris, John Parthenios, Nicola Pugno, Konstantinos Papagelis, Kostya S. Novoselov and Costas Galiotis,
NPG Scientific Reports 4, 5271 (2014), **OPEN ACCESS**
DOI: 10.1038/srep05271

17. Towards Efficient Drug Delivery Trough Suitably Prepared Metal-Organic-Frameworks: A First Principle Study,
Emmanuel N. Koukaras, Tamsyn Montagnon, Pantelis Trikalitis, Dimitrios Bikiaris, Aristides D. Zdetsis, George E. Froudakis,
ACS Journal of Physical Chemistry C 118, 8885–8890 (2014)
DOI: 10.1021/jp410282m

16. Size Dependence of the Structural, Electronic, and Optical Properties of $(CdSe)_n$, n=6–60, Nanocrystals,
Aristides Zdetsis, Michael M. Sigalas and Emmanuel Koukaras,
RSC Advances 4, 14613–14623 (2014)
DOI: 10.1039/C4RA00966E

15. Properties and energetics for design and characterization of chitosan nanoparticles used for drug encapsulation,
Emmanuel N. Koukaras, Sofia A. Papadimitriou, Dimitrios N. Bikiaris, George E. Froudakis,
RSC Advances 4, 12653–12661, (2014)
DOI: 10.1039/C3RA47572G

14. Dye-sensitized solar cells based on triazine-linked porphyrin dyads containing one or two carboxylic acid anchoring groups,
Galateia E. Zervaki, Panagiotis A. Angaridis, Emmanuel N. Koukaras, Ganesh D. Sharma and Athanassios G. Coutsolelos,
RSC Inorganic Chemistry Frontiers 1, 256 (2014)
DOI: 10.1039/C3QI00095H

13. New conjugated alternated benzodithiophene-containing copolymers with different acceptor units: synthesis and photovoltaic application,
G. D.Sharma, V. S. Kochurov, D. V. Marochkin, A. R. Khokhlov and E. N. Koukaras,
RSC Journal of Materials Chemistry A 2, 155–171, (2013)
DOI: 10.1039/C3TA12967E

12. Synthesis and characterization of two carbazole-based alternating copolymers with 4-nitrophenylcyanovinylene pendant groups and their use as electron donors for bulk heterojunction solar cells,
G. D. Sharma, Manjeet Singh, Rajnish Kurchania, E. N. Koukaras, and J. A. Mikroyannidis,
RSC Advances 3,18821–18834 (2013)
DOI: 10.1039/c3ra42299b

11. Size dependence of the optical gap of "small" silicon quantum dots: *Ab Initio* and empirical correlation schemes,
Shanawer Niaz, Emmanuel N. Koukaras, Nikolaos P. Katsougrakis, Theodoros G. Kourelis, Dimitrios K. Kougias, and Aristides D. Zdetsis,
Elsevier Microelectronic Engineering 112, 231–234 (2013)
DOI: 10.1016/j.mee.2013.07.005

10. Synthesis and characterization of low band gap quinoxaline based D−A copolymer and its application as donor for bulk heterojunction polymer solar cells,
M. L. Keshtov, D. V. Marochkin, V. S. Kochurov, A. R. Khokhlov, E. N. Koukaras, and G. D. Sharma,

RSC Polymer Chemistry 4, 4033–4044 (2013)
DOI: 10.1039/C3PY00391D

9. Theoretical study of oxygen contaminated silicon quantum dots: A case study for $Si_{29}H_{29-x}O_{29-y}$,
Aristides D. Zdetsis, Shanawer Niaz, and Emmanuel N. Koukaras,
Elsevier Microelectronic Engineering 112, 227–230 (2013)
DOI: 10.1016/j.mee.2013.05.008

8. *Ab initio* study of Magnesium and Magnesium hydride nanoclusters and nanocrystals: Examining optimal structures and compositions for efficient hydrogen storage,
Emmanuel N. Koukaras, Aristides D. Zdetsis, Michael M. Sigalas,
ACS Journal of the American Chemical Society (JACS) 134, 15914–15922 (2012)
DOI: 10.1021/ja306344b

7. Insight on the Formation of Chitosan Nanoparticles through Ionotropic Gelation with Tripolyphosphate,
Emmanuel N. Koukaras, Sofia A. Papadimitriou, Dimitrios N. Bikiaris, and George E. Froudakis,
ACS Molecular Pharmaceutics 9, 2856–2862 (2012)
DOI: 10.1021/mp300162j

6. Phononic bandgaps in graphene-based materials,
Michael M. Sigalas and Emmanuel N. Koukaras,
AIP Applied Physics Letters 100, 203109 (2012)
DOI: 10.1063/1.4717746

5. Structural and Static Electric Response Properties of Highly Symmetric Lithiated Silicon Cages: Theoretical Predictions,
E. N. Koukaras, A. D. Zdetsis, P. Karamanis, C. Pouchan, A. Avramopoulos and M. G. Papadopoulos,
ACS Journal of Computational Chemistry 33, 1068–1079 (2012)
Selected for the Issue 10 (15 April 2012) **Cover Article.**
DOI: 10.1002/jcc.22938

4. Theoretical Study of Amino Acid Interaction with Metal−Organic Frameworks,
E. N. Koukaras, A. D. Zdetsis, and G. E. Froudakis,
ACS Journal of Physical Chemistry Letters 2, 272–275 (2011)
DOI: 10.1021/jz101602p

3. Multidecker sandwiches of silicon–carbon clusters**,**
E. N. Koukaras and A. D. Zdetsis,
ACS Organometallics 28 (15), 4308–4315 (2009)
DOI: 10.1021/om9003253

2. Structural properties and magic structures in hydrogenated finite and infinite silicon nanowires,
A. D. Zdetsis, E. N. Koukaras, and C. S. Garoufalis,
AIP Applied Physics Letters 91, 203112, (2007)
DOI: 10.1063/1.2813019

1. Structure and properties of the $Ni@Si_{12}$ cluster from all-electron *ab initio* calculations,
E. N. Koukaras, C. S. Garoufalis, and A. D. Zdetsis,
APS Physical Review B 73, 235417 (2006)
DOI: 10.1103/PhysRevB.73.235417

B. International Conference Proceedings — ISI-indexed — Peer Reviewed

12. Theoretical study of $Si_{20}Li_{20}$ cage clusters,
Aristides D. Zdetsis and Emmanuel N. Koukaras,
ICCMSE 2009 – International Conference of Computational Methods in Sciences and Engineering, Rhodes, Greece, 29 September–4 October 2009
AIP Conference Proceedings 1504, 683–686 (2012)
DOI: 10.1063/1.4771787

11. *Ab initio* study of the Silicon-Bismuth interface: Bismuth nanolines and Bismuth-covered Silicon nanoparticles,
A. D. Zdetsis, E. N. Koukaras, and D. A. Zdetsis,
4th International Conference on Micro-Nanoelectronics, Nanotechnologies & MEMs, NCSR Demokritos, Athens, Greece, 12–15 December 2010
Microelectronic Engineering 90, 99–103 (2011)
DOI: 10.1016/j.mee.2011.05.031

10. Theoretical study of the elasticity of ultra-thin finite silicon nanowires. I. Semiempirical model considerations,
E. N. Koukaras, S. Niaz, D. A. Zdetsis, and A. D. Zdetsis,
4th International Conference on Micro-Nanoelectronics, Nanotechnologies & MEMs, NCSR Demokritos, Athens, Greece, 12–15 December 2010
Microelectronic Engineering 90, 88–91 (2011)
DOI: 10.1016/j.mee.2011.04.042

9. A systematic way for obtaining the structural and electronic properties of silicon–carbon clusters of the form Si_nC_2, n=1–5,
E. N. Koukaras, M. Mühlhäuser and A. D. Zdetsis,
ICCMSE 2008 – International Conference of Computational Methods in Sciences and Engineering, Hersonissos, Crete, 25–30 September 2008
AIP Conference Proceedings 1148, 384 (2009)
DOI: 10.1063/1.3225323

8. Multidecker stacking and cluster fusion of silicon–carbon clusters,
E. N. Koukaras and A. D. Zdetsis,
ICCMSE 2008 – International Conference of Computational Methods in Sciences and Engineering, Hersonissos, Crete, 25–30 September 2008
AIP Conference Proceedings 1148, 368 (2009)
DOI: 10.1063/1.3225318

7. Elastic properties of ultra-thin hydrogenated silicon nanowires based on all electron mixed ab initio and semiempirical calculations,
E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis,
ICCMSE 2008 – International Conference of Computational Methods in Sciences and Engineering, Hersonissos, Crete, 25–30 September 2008

AIP Conference Proceedings 1148, 376 (2009)
DOI: 10.1063/1.3225320

6. A parallel study of Ni@Si_{12} and Cu@Si_{12} nanoclusters,
A. D. Zdetsis, E. N. Koukaras and C. S. Garoufalis,
ICCMSE 2005 – International Conference of Computational Methods in Sciences and Engineering, Loutraki, Korinthos, Greece, 21 – 26 October 2005
Springer Journal of Mathematical Chemistry 46, 971 (2009)
DOI: 10.1007/s10910-009-9549-x

5. Mixed silicon-germanium nanocrystals: A detailed study of Si_xGe_{47-x}:H,
A. D. Zdetsis, C. S. Garoufalis, and E. N. Koukaras,
ICCMSE 2005 – International Conference of Computational Methods in Sciences and Engineering, Loutraki, Korinthos, Greece, 21 – 26 October 2005
Springer Journal of Mathematical Chemistry 46, 942 (2009)
DOI: 10.1007/s10910-009-9555-z

4. Novel effects in finite-length silicon nanowires**,**
A. D. Zdetsis, E. N. Koukaras, and C. S. Garoufalis,
3rd International Conference on Micro-Nanoelectronics, Nanotechnology and MEMs (Micro & Nano 2007), Athens, Greece, 18 – 21 November 2007
Wiley Physica Status Solidi (a) 205, 2625, (2008)
DOI: 10.1002/pssa.200780159

3. High-stability finite-length silicon nanowires: A real space theoretical study,
E. N. Koukaras, A. D. Zdetsis and C. S. Garoufalis,
ICCMSE 2007 – International Conference of Computational Methods in Sciences and Engineering, Corfu, Greece, 25 – 30 September 2007
AIP Conference Proceedings 963, 375 (2007)
DOI: 10.1063/1.2836089

2. Electronic and structural properties of M@Si_{12} and M@$Si_{12}H_{12}$ clusters, M = Ni, Zn,
E. N. Koukaras and A. D. Zdetsis,
ICCMSE 2007 – International Conference of Computational Methods in Sciences and Engineering, Corfu, Greece, 25 – 30 September 2007
AIP Conference Proceedings 963, 395 (2007)
DOI: 10.1063/1.2836094

1. Variation and adjustment of the optical gap of small Si nanocrystals by partial substitution of Si with Ge,
A. D. Zdetsis, C. S. Garoufalis, M. S. Skaperda and E. N. Koukaras,
2nd Conference on Microelectronics, Microsystems and Nanotechnology, Athens, Greece, 14–17 November 2004
Journal of Physics: Conference Series 10, 101 (2005)
DOI: 10.1088/1742-6596/10/1/025

BI. International Conference Proceedings — ISI-indexed — Not Peer Reviewed

3. Compression behaviour of embedded graphenes of various thicknesses,
Galiotis, C., Androulidakis, Ch., Koukaras, E. N., Parthenios, J., Papagelis, K.

ECCM17 – 17th European Conference on Composite Materials, Munich, Germany, 26 – 30 June 2016

2. Compression behavior of graphene flakes of various thicknesses embedded into polymer matrices,
   John Parthenios, Charalampos Androulidakis, Emmanuel N. Koukaras, Georgia Tsoukleri, Dimitris Sfyris, Konstantinos Papagelis, and Costas Galiotis,
   ICCM20 – 20th International Conference on Composite Materials, Copenhagen, 19 – 24 July 2015
1. Compression failure of graphene sheets in polymer nanocomposites,
   Charalampos Androulidakis, Emmanuel N. Koukaras, Otakar Frank, Georgia Tsoukleri, Dimitris Sfyris, John Parthenios, Nicola Pugno, Konstantinos Papagelis, Kostya S. Novoselov, and Costas Galiotis,
   ECCM16 – 16th European Conference on Composite Materials, Seville, Spain, 22–26 June 2014

BN. International Conference Proceedings — Not ISI-indexed

11. On the Mechanical Response of Graphene Ribbons Under Strain,
    E. N. Koukaras, Ch. Androulidakis, M. Hadjinicolaou, and C. Galiotis,
    Graphene Week 2017, Athens, Greece, 25 – 29 September 2017
10. Interfacing graphene to compliant polymer: wrinkles and stress transfer,
    Charalampos Androulidakis, Emmanuel N. Koukaras, Jaroslava Rahova, Krishna Sampathkumar, John Parthenios, Konstantinos Papagelis, Otakar Frank and Costas Galiotis,
    Graphene Week 2017, Athens, Greece, 25 – 29 September 2017
9. Compression behaviour of embedded graphene of various thicknesses,
   Ch. Androulidakis, Emmanuel N. Koukaras, G. Tsoukleri, D. Sfyris, J. Parthenios, I. Polyzos, K. Papagelis and C. Galiotis,
   Graphene Week 2015, Manchester, UK, 22 – 26 June 2015
8. Compression instabilities of graphene flakes of various thicknesses embedded into polymer matrices,
   Costas Galiotis, Ch. Androulidakis, E. N. Koukaras, G. Tsoukleri, D. Sfyris, I. Polyzos, J. Parthenios, K. Papagelis,
   Graphene Week 2015, Manchester, UK, 22 – 26 June 2015
7. Effect of number of layers on the compression behaviour of graphenes,
   Ch. Androulidakis, E. N. Koukaras, G. Tsoukleri, D. Sfyris, I. Polyzos, J. Parthenios, K. Papagelis, and C. Galiotis,
   GraphITA 2015, Bologna, Spain, 14 – 18 September 2015
6. Mechanical behaviour of embedded monolayer graphene sheets under axial loading,
   C. Galiotis, Ch. Androulidakis, E. Koukaras, Otakar Frank, G. Tsoukleri, D. Sfyris, J. Parthenios, K. Papagelis,
   Graphene 2014, Toulouse, France, 6 – 9 May 2014
5. *Ab initio* study of electronic and structural properties of the $Ni@Si_{10}$ cluster,
   E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis,
   ICCMSE 2006 – International Conference of Computational Methods in Sciences and Engineering, Chania, Crete, Greece, 27 October – 1 November 2006
   Lecture Series on Computer and Computational Sciences 7B, 1174, Brill Academic Publishers, eds. T. Simos and G. Maroulis (2006)
4. *Ab initio* study of optical and electronic properties of silicon and germanium nanowires,

E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis,
ICCMSE 2006 – International Conference of Computational Methods in Sciences and Engineering, Chania, Crete, Greece, 27 October – 1 November 2006
Lecture Series on Computer and Computational Sciences 7B, 1182, Brill Academic Publishers, eds. T. Simos and G. Maroulis (2006)

3. A comparative DFT and MP*n* study of isoelectronic $[Co@Si_{12}]^{-1}$, $[Ni@Si_{12}]$ and $[Cu@Si_{12}]^{+1}$ clusters,
A. D. Zdetsis, E. N. Koukaras and C. S. Garoufalis,
ICCMSE 2006 – International Conference of Computational Methods in Sciences and Engineering, Chania, Crete, Greece, 27 October – 1 November 2006
Lecture Series on Computer and Computational Sciences 7B, 1178, Brill Academic Publishers, eds. T. Simos and G. Maroulis (2006)
2. Structural and electronic properties of the $Ni@Si_{12}$ nanocluster,
E. N. Koukaras, C. S. Garoufalis and A. D. Zdetsis,
ICCMSE 2005 – International Conference of Computational Methods in Sciences and Engineering, Loutraki, Korinthos, Greece, 21 – 26 October 2005
Lecture Series on Computer and Computational Sciences, 4, 1492 (2005)
1. Optical and electronic properties of mixed SiGe:H nanocrystals,
A. D. Zdetsis , C. S. Garoufalis and E. N. Koukaras,
ICCMSE 2005 – International Conference of Computational Methods in Sciences and Engineering, Loutraki, Korinthos, Greece, 21 – 26 October 2005
Lecture Series on Computer and Computational Sciences, 4, 1488 (2005)

C. National Conference Proceedings

10. Single layer graphene flakes under tension and its failure process under compressive loadings,
Ch. Androulidakis, Emmanuel N. Koukaras, G. Tsoukleri, D. Sfyris, J. Parthenios, K. Papagelis and C. Galiotis,
10th Hellenic Polymer Society Conference, Patra, Greece, 4 – 6 Dec 2014
9. Towards a thorough understanding of stress transfer mechanisms at the sub-micron level,
G. Anagnostopoulos, Ch. Androulidakis, G. Tsoukleri, E. N. Koukaras, I. Polyzos, J. Parthenios, K. Papagelis and C. Galiotis,
10th Hellenic Polymer Society Conference, Patra, Greece, 4 – 6 Dec 2014
8. Computational modelling of nanoporous materials for sustainable energy and environmental applications
I. Skarmoutsos, E. Klontzas, E. Koukaras, G. Maurin
ΠΕΣΧΜ 2019 – 12ο Πανελλήνιο Συνέδριο Χημικής Μηχανικής, Πάτρα, 4–6 Ιουνίου 2015
URL: https://12pesxm.chemeng.ntua.gr/view_author/63
7. Structural, electronic and mechanical properties of molecularly pillared, 3D nanoporous graphene materials
Ε. Κλώντζας, Γ. Ε. Φρουδάκης, Ι. Σκαρμούτσος, Κ. Γαλιώτης, Ε. Ν. Κουκάρας
ΠΕΣΧΜ 2019 – 12ο Πανελλήνιο Συνέδριο Χημικής Μηχανικής, Πάτρα, 4–6 Ιουνίου 2015
URL: https://12pesxm.chemeng.ntua.gr/view_author/63
6. On the compression behaviour of multilayer graphene flakes embedded in gel matrices
Charalampos Androulidakis, Emmanuel N. Koukaras, Ioannis Polyzos, John Parthenios, Konstantinos Papagelis, and Costas Galiotis

ΠΕΣΧΜ 2015 – 10ο Πανελλήνιο Συνέδριο Χημικής Μηχανικής, Πάτρα, 4–6 Ιουνίου 2015
URL: http://pesxm10.chemeng.upatras.gr/all-authors-alpabetical/%CE%BA?page=4

5. Modeling and Theoretical Studies of Graphene at Multiple Scales
G. Kalosakas, N.N. Lathiotakis, E.N. Koukaras, D. Sfyris, C. Galiotis and K. Papagelis
10η Επιστημονική Διημερίδα του ΙΤΕ, Ηράκλειο, Κρήτη, 12–13 Ιουλίου 2013
URL: https://www.forth.gr/index_main.php?l=g&c=18&i=454

4. *Ab initio* investigation of the interaction of glycine and other amino acids with Metal–Organic-Frameworks (MOFs),
E. N. Koukaras, A. D. Zdetsis, and G. E. Froudakis.
XXVI Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα (2010).
3. Organometallic Multidecker silicon-carbon sandwiches,
E. N. Koukaras and A. D. Zdetsis.
XXVI Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα (2010).
2. Exploring the possibility of drug delivery for cancer therapy through carbon-boron and carbon-silicon nanorods,
E. N. Koukaras, N. Katsougrakis, T. Kourelis, and A. D. Zdetsis.
XXVI Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα (2010).
1. Θεωρητικοί υπολογισμοί οπτικού χάσματος σε κβαντικές «κηλίδες» γερμανίου και γερμανίου–πυριτίου.
Μ. Σκαπέρδα, Χ. Σ. Γαρουφαλής, Ε. Κουκάρας και Α. Δ. Ζδέτσης.
ΧΧ Πανελλήνιο Συνέδριο Φυσικής Στερεάς Κατάστασης, Ιωάννινα (2004).