Michael P. Sigalas

Assistant Professor/Associate Professor/Professor

LAB OF QUANTUM AND COMPUTATIONAL CHEMISTRY, DEPARTMENT OF CHEMISTRY, ARISTOTLE UNIVERSITY OF THESSALONIKI

sigalas@chem.auth.gr
ORCID: 0000-0002-4166-2057
Google scholar:
https://scholar.google.com/citations?user=fYbxjOIAAAAJ&hl=el&oi=sra
(citations: 2215, h-index: 25)
SCOPUS: 7006137176
Tel.: 6945386850
Website: https://www.chem.auth.gr/staff/sigalas/

EDUCATION

1980   Bachelor of Chemistry, DEPARTMENT OF CHEMISTRY, ARISTOTLE UNIVERSITY OF THESSALONIKI

1984   PhD, DEPARTMENT OF CHEMISTRY, ARISTOTLE UNIVERSITY OF THESSALONIKI

RESEARCH FIELDS

- Quantum Chemical Study of the Molecular Structure
- Computational Chemistry
- Information na communication Technology in Chemical Education
- Design and Developement of Educational Software and Multimedia Material of Chemistry

EDUCATIONAL EXPERIENCE

UNDERGRADUATE COURSES

➢   Principles of Quantum Chemistry and Spectroscopy/Mandatory
➢   Applied Mathematics to Chemistry I/Selection
➢   Applied Mathematics to Chemistry II/Selection
➢   Real, virtual and hybrid laboratories/selection
➢   Computational Chemistry/Selection
➢   Molecular modeling/selection
➢   Construction, presentation and dissemination of chemical information/selection
➢   Development of multimedia chemistry material and teaching using telecommunications networks /selection
➢   Molecular symmetry and group/selection

GRADUATE COURSES

➢   Department of Chemistry,AUTH/Postgraduate Program: 'MOLECULAR DESIGN AND MODELING-CHEMICAL EDUCATION'/Molecular Properties/Quantum chemical Study of Chemical Reactivity/Teaching Approach to Chemistry Subjects/Information and Communication Technologies, Techniques and development tools for the visualization of the molecular structure, chemical properties and data.

➢   Department of Chemistry of EKPA/Postgraduate Program: "ΔιΧηNET-EAA"/Methodology and tools for visualization of the molecular structure, chemical properties and data.

DISCRIMINATIONS / SCHOLARSHIPS

➢ *MERLOT Classics Award* for Exemplary on-line educational Chemistry software from the Chemistry Committee of *MERLOT organization (Multimedia Educational Resources for Learning and Online Teaching)* for the software *«3DMolSym»*, (N.D. Charistos, M.P. Sigalas), Mineapolis, USA, 2008.

➢ *Innovation Award* for the research group "MolWave" of the Department of Chemistry for the development of educational Software (L. Antonoglou, V. Koutalas, N.D. Charistos, M.P. Sigalas), Research Commitee AUTH, 2009.

➢ *Award of Excellence* for the research group "MolWave" of the Department of Chemistry for the development of educational Software (L. Antonoglou, V. Koutalas, N.D. Charistos, M.P. Sigalas), Ministry of Education, 2011.

RESEARCH GRANTS

PI for the following research programs

➢ "Educational approach of Chemistry concepts and phenomena and development of software and multimedia material for their effective teaching/General Secretariat of Research and Technology /1991-1994.

➢ "Theoretical Study of the effect of the change of coordination number and geometry on the catalytics ability of complex compounds"/ Ministry of industry, research and technology, Ministries of Interior affairs, Education, Research, Technology and Environment of France/1993-1995.

➢ «Organization and Running of the Interuniversity – interdepartment Graduate Program "Didactics of Chemistry and New Educational Technologies" (ΔιΧηΝΕΤ)/ Υπουργείο Παιδείαw/1997-2004.

➢ "Training in Chemistry of professors of Secondary Education"/ Ministry of education /1999-2001.

➢ «Preparation of the Information Society Teacher/Initial training of all educators in the Technologies of Informatics and Communication» / Ministry of education /2002-2003.

➢ "Upgrade and modernization of the Graduate Program of the Department of Chemistry "/ Ministry of education /1997-2000.

➢ "Upgrade of the Graduate Program and the educational procedures of the Department of Chemistry with the enhancement of laboratory exercise of students, the introduction of new educational technologies and of the continuous assessment of the educational procedure"/ Ministry of education /2001-2006.

➢ "Development of supportive e-material for the lesson of Chemistry in high school"/ Pedagogical Institute/2003-2005.

➢ "Pleiades: Development of Educational Software and Integrated Educational Packages for Greek Schools of Primary and Secondary Education & Educational Software Products in Schools - Nereides: Development of Integrated Educational Packages. Carbon B "/EAITY/2006-2007.

➢ "Pleiades: Development of Educational Software and Integrated Educational Packages for Greek Schools of Primary and Secondary Education & Educational Software Products in Schools - Nereides: Development of Integrated Educational Packages. Chemical calculations B "/EAITY/2006-2007.

➢ "Teacher training in the use and utilization of ICTs in the educational teaching process/ Ministry of education /2007—2009.

➢ «Visuospatial abilities of students and understanding - learning of concepts related to the molecular structure. Design, development and evaluation of molecular visualization and augmented reality software for secondary and higher education»/ Ministry of education /2011-2015.

REVIEWER OF SCIENTIFIC JOURNALS

• "Chemical Physics"

• "Journal of Computational Chemistry"

• "Journal of Molecular Modeling, THEOCHEM"

• "Journal of Physical Chemistry, A"

• "Journal of Molecula Modeling"

• "Journal of Computational Methods in Science and Engineering"

• "New Journal of Chemistry"

• "Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy"

• "Inorganic Chemistry"

- "Inorganic Chemistry Communications"
- "Journal of Coordination Chemistry"
- "Chemistry Education: Research and Practice in Europe"
- "Journal of Chemical Education"
- "Journal of Chemical Education: Software"
- "Journal of Chemical Education: Internet"
- "Computers and Education"

EDITOR OF BOOKS AND SPECIAL VOLUMES

(1) "The HMO Model. Theory and Applications"
C.A. Tsipis, M.P. Sigalas and E.G. Bakalbasis, Thessaloniki, 1990.
(2) "Physical Methods in Inorganic Chemistry. Normal Coordinate Analysis"
M.P. Sigalas, Thessaloniki, 1993.
(3) "Development of Multimedia Applications with Macromedia Director"
M.P. Sigalas and N. D. Charistos, Thessaloniki, 1993.
(4) "Design of Molecular Visualization Educational Software for Chemistry Learning"
L.D. Antonoglou, N.D. Charistos and M.P. Sigalas, In "Leading-Edge Educational Technology", Nova Publishers, 2008.
(5) "Computational Chemistry" [e-book]
M.P. Sigalas,Thessaloniki, 2014.
(6) "Molecular Symmetry and Group Theory. Principles and Applications"[e-book]
M.P. Sigalas, L.D. Antonoglou and N.D. Charistos. Athens, 2016.
(https://repository.kallipos.gr/handle/11419/4019)
(7) Exploring Chemistry Problems with Computational Quantum Chemistry Tools in the Undergraduate Chemistry Curriculum, M.P. Sigalas, In "Problems and Problem Solving in Chemistry Education: Analysing Data, Looking for Patterns and Making Deductions", RSC, 2021.

PATENTS

ADDITIONAL INFORMATION

- Presentations at conferences: **100**
- Supervision of doctoral theses: **7**
- Supervision of graduate students: **50**
- Supervision of undergraduate students: **20**
- Reviewer in Research Programs: **1**

SELECTED PUBLICATIONS (link OF PUBLICATIONS)

~110 publications (https://scholar.google.com/citations?user=fYbxjOIAAAAJ&hl=el&oi=sra)

10 selected recent publications
The balance between side-chain and backbone-driven association in folding of the α-helical influenza A transmembrane peptide
I Stylianakis, A Shalev, S Scheiner, MP Sigalas, IT Arkin, N Glykos, ...
Journal of Computational Chemistry 41 (25), 2177-2188   4   2020

Polyaromatic Systems Combining Increasing Optical Gaps and Amplified Nonlinear Optical Properties. A Comprehensive Theoretical Study on B3N3 Doped …
P Karamanis, ND Charistos, MP Sigalas, M Rérat
The Journal of Physical Chemistry C 123 (34), 21135-211499   2019

The pseudo-π model of the induced magnetic field: fast and accurate visualization of shielding and deshielding cones in planar conjugated hydrocarbons and spherical fullerenes
ND Charistos, A Munoz-Castro, MP Sigalas
Physical Chemistry Chemical Physics 21 (11), 6150-6159   12   2019

Canonical orbital contributions to the magnetic fields induced by global and local diatropic and paratropic ring currents
ND Charistos, AG Papadopoulos, TA Nikopoulos, A Muñoz-Castro, ...
Journal of Computational Chemistry 38 (30), 2594-2604   16   2017

Changes in visual/spatial and analytic strategy use in organic chemistry with the development of expertise
M Vlacholia, S Vosniadou, P Roussos, K Salta, S Kazi, M Sigalas, ...
Chemistry Education Research and Practice 18 (4), 763-773   12   2017

DFT study of radical scavenging activity of sesame oil lignans and selected in vivo metabolites of sesamin
AG Papadopoulos, N Nenadis, MP Sigalas
Computational and Theoretical Chemistry 1077, 125-132   16   2016

Study of Electron Delocalization in 1, 2-, 1, 3-, and 1, 4-Azaborines Based on the Canonical Molecular Orbital Contributions to the Induced Magnetic Field and Polyelectron …
AG Papadopoulos, ND Charistos, K Kyriakidou, MP Sigalas
The Journal of Physical Chemistry A 119 (39), 10091-10100   20   2015

Unusual coordination mode of 3-methoxysalicylaldehyde in mononuclear zinc (II) complexes with nitrogenous bases
D Anastasiadou, E Coutouli-Argyropoulou, M Gdaniec, A Czapik, ...
Polyhedron 87 (IKEEXREF-271605), 275-285   6   2015

Investigating the Visual/Analytic Shift in Students' Knowledge in Chemistry.
M Vlacholia, S Vosniadou, K Salta, P Roussos, S Kazi, MP Sigalas, ...
CogSci   1   2015

Interaction of Chromium(III) with a N,N'-Disubstituted Hydroxylamine-(diamido) Ligand: A Combined Experimental and Theoretical Study
PA Tziouris, CG Tsiafoulis, M Vlasiou, HN Miras, MP Sigalas, ...
Inorganic Chemistry 53 (21), 11404-11414   2014