europass

Vangelis Daskalakis

Date of birth: 24/12/1978 | **Nationality:** Greek | **Gender:** Male | **Phone number:** (+30) 6942436906 (Mobile) | **Phone number:** (+30) 2610997820 (Work) | **Email address:** vdaskalakis@upatras.gr | **Email address:** vdaskalakis@iceht.forth.gr | **ORCID:** https://orcid.org/0000-0001-8870-0850 |

Address: University of Patras, Greece, Caratheodory 1, University Campus, GR 265 04, Patras, Greece (Work)

ABOUT ME

place of birth / Heraklion, Crete-Greece

WORK EXPERIENCE

DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS – PATRAS, GREECE

Address Caratheodory 1, University Campus, GR 265 04, Patras, Greece

ASSISTANT PROFESSOR – 01/09/2023 – CURRENT

Biomolecular Engineering (ΦΕΚ 693/13-3-2023 τ.Γ')

Research Grants:
1. (2025-2026) Proposal No. EHPC-EXT-2025E01-070 **EuroHPC Extreme Scale Access Call** "Digital zoom into the All-atom dynamics of Light-harvesting complexes (DALiA)", 255160 node hours or **20.412.800 core hours MareNostrum5 ACC** (**Accelarated Partition**). PI: Vangelis Daskalakis
2. (2025-2026) Proposal No. EHPC-REG-2025R01-105 **EuroHPC Regular Access Call** "Decoding the Disorder and Promiscuity of Sec14-like SFH Proteins Through Molecular Dynamics (SECure)", 230000 node hours or **25.760.000 CPU-core hrs MareNostrum5 GPP (General Purpose Partition)**. PI: Vangelis Daskalakis
3. (2025) **NAISS** Medium Compute 2025 project (Sweeden) NAISS 2025/5-204 "Sampling the configuration assembly of SFH8 through molecular dynamics", **485300 CPU-core hrs** at Tetralith @ NSC, PI: Panagiotis Nikolaou Moschou.
4. (2024-2028) Horizon Europe (HORIZON) Marie Skłodowska-Curie Actions Doctoral Networks (MSCA-DN) 2022, **101119442-PhotoCaM** - "*Photosynthetic Antennas in a Computational Microscope: Training a new generation of computational scientist*" (total budget: ***€2.589.847,19****, vice-Coordinator* UPAT ***€240.098,39****;* PI: Vangelis Daskalakis).
5. (2024-2025) Hellenic Foundation for Research and Innovation (H.F.R.I.) proposal No. 14775 SA3. Life Sciences, "SUNDIAL - Seeing Diatoms under a Computational Sunlight". *Coordinator* UPAT ***€207.000****;* PI: Vangelis Daskalakis
6. (2023-2024) Cyclone 2022A Production Access: **pro22a103s1** - "*Fucoxanthin - chlorophyll protein (FCP): from monomers to tetramers*", **150.000 GLU-core hrs** on Cyclone. PI: Vangelis Daskalakis
7. (2023-2024) Proposal No. EHPC-REG-2023R01-128 **EuroHPC Regular Access Call** "*Peptaibols*: *How to kill a bacterium*", **6.400.000 CPU-core hrs** on MeluXina. PI: Vangelis Daskalakis
8. (2024-2026) 16-18th Calls for Production Projects Accessing ARIS HPC:
(a) FCPC - Water/ Proton Conductance in the FCP Light Harvesting Complexes of Diatoms (PI, 1.000.000 GPU core-hrs)
(b) GemT – Molecular dynamics of bacterial gemcitabine transporters (collaborator, 2.000.000 CPU core-hrs)
(c) MultiEng: Engineering multifunctional biocatalysts for the valorization of lignocellulosic biomass (collaborator, 1.500.000 CPU core-hrs)
(d) PscAC: PscA-PscC dynamics in the green sulfur bacteria photosynthetic machinery (collaborator, 700.000 GPU core-hrs)
(e) FanPath: Allosteric Communication and R-Loop Dynamics in Eukaryotic RNA-Guided Nucleases (PI, 1.500.000 core hrs GPU node island)

UNIVERSITY OF PATRAS – PATRAS, GREECE

VISITING FACULTY MEMBER AT FORTH/ICE-HT – 07/03/2025 – CURRENT

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

DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY – LIMASSOL, CYPRUS

ASSOCIATE PROFESSOR – 01/05/2022 – 31/08/2023

Research/ Grants:
1. European High-Performance Computing Joint Undertaking (**EuroHPC JU**) project **EHPC-REG-2021R0021** "*Peptaibols: How to kill a bacterium*", at MeluXina supercomputer (Luxembourg), 2.0 mn std-cpu-core hrs, coordinator (**Apr 2022 - Oct 2022**).
2. Erasmus+ Learning Mobility of Individuals – Staff mobility for teaching and training activities, Queen Mary University of London (**May 2022**)

DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY – LIMASSOL, CYPRUS

ASSISTANT PROFESSOR – 31/12/2014 – 30/04/2022

Research/ Grants:
1. 13th Allocation **Cyclone** (**The Cyprus Institute**) project CfP13 - "Molecular Dynamics of LHCII trimer complex at quenched and light harvesting states based on Free Energy Minima" (~1.0mn std-cpu core hrs), as coordinator (**Apr 2021 – March 2022**).
2. **GRnet 10th Call** ARIS project CYP2D6-DYN "Correlation between CYP2D6 variants and their metabolic activity by Molecular Dynamics Simulations" (3.5mn std-cpu core hrs), as collaborator (**March 2021 – Feb 2022**)
3. **PRACE DECI-16 16DECI0015 DynLHCX** "The structure and dynamics of the photoprotective protein LHCX1 in diatoms", 5.0mn std-cpu core hrs, as coordinator (**June 2020 – May 2021**)
4. **PRACE COVID-19 COVID19-41** "Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution", 18.0mn std-cpu core hrs @Joliot-Curie Rome (CEA/GENCI, France) (**May 2020 – Nov 2021**)
5. COST Action CA18234: "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements", Management Committee MC member (**April 2020 – 2024**), WP2 Molecular Dynamics Simulations member.
6. **PRACE DECI-15 15DECI0328 LHCPSSalt** "LHCII-PsbS complex conformations under varying salt content" ~4.0mn std-cpu core hrs, as coordinator (**June 2019 – May 2020**).
7. **PRACE Project 2018194641** 17.0mn std-cpu core hrs @SuperMUC HPC (Leibniz Supercomputing Centre). "CDynLHCII - Clustering Dynamics of the major Light Harvesting Complexes (LHCII) of Photosystem II under Photoprotection", as coordinator (**April 2019 – March 2020**).
8. Cyprus Research Promotion Foundation project **POST-DOC/0916/0049** "*Triggering Photoprotection in Photosystem II Antenna by Molecular Simulations and Raman Spectroscopy*" (~160.000 Euros), as coordinator (**Oct 2018 – March 2022**).
9. Interreg Greece-Cyprus, BIOMA «*Decentralized management of bio-waste and their exploitation through the use of alternative and innovative treatment systems*».
10. HPC-Europa3 Transnational Access programme (HPC17K4FRZ, 672.000 std cpu-core hrs) (2018) and Research Training Group Quantum Mechanical Materials Modelling (TRG-qm3, 2019) during Sabbatical Leave. Department of Physics & Earth Sciences (Biophysics Group), Jacobs University, Bremen, Germany (**Sept 2018 – Feb 2019**).
11. Cy-Tera-LinkSCEEM, PRACE HPC, GRnet ARIS Grants ~7.0mn total cpu standard core-hours for projects: pro14b114s1, pro14b105s1 and pro15a113s1, pro15b104, pro16a105, pro16b103, pro17a103, pro17b101, lspre400, lspre410, **PRACE DECI-13** LHCFlex, **PRACE DECI-14** AIMDPSII, GRnet preparatory ARIS "ADHDyn" & "LHCIIPsbS" as PI/ coordinator. **GRnet 7th Call for Production** Projects Accessing ARIS project "LHCIICRYSTAL" 3.0 mn std cpu-core hrs, *as collaborator*.
12. COST Action CM1401: Our Astro-Chemistry History. Management Committee MC member (start April 2015).
13. Erasmus Grant Mobility for Training (visitor to the Academy of Sciences of the Czech Republic, Institute of Organic Chemistry and Biochemistry, Prague). May 2015.

DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY – LIMASSOL, CYPRUS

LECTURER – 30/11/2010 – 30/12/2014

Research/ Grants:
1. Startup Grant Cyprus University of Technology (40.000 €)
2. "Activation and reduction of Nitric Oxide (NO) to laughing gas (N_2O) by Nitric Oxide Reductase (NOR) and heme-copper cbb_3 oxidase (financial entity: Cyprus Research Promotion Foundation €133.181. Technology/ΘΕΠΙΣ/0609/05 (BE): (2011-2013) as a collaborator (**March 2011 – Feb 2013**).
3. Cy-Tera & LinkSCEEM HPC Preparatory Access and Production Grants (860.000 total cpu standard core-hours, for projects: LinkSCEEM lsprob104s1, lspro13a121s1, pro13b113s1, and pro14a120) as coordinator.
4. The Deutscher Akademischer Austauschdienst (DAAD)/ German Academic Exchange Service Grant for ASEMUNDUS Networking Programme (Collaboration between Universities in Asia-Europe).
5. COST Action ES1206: Advanced Global Navigation Satellite Systems tropospheric products for monitoring severe weather events and climate (GNSS4SWEC) – Management Committee & WG2 member (terminated April 2015).

LIFE SCIENCES DEPARTMENT, BARCELONA SUPERCOMPUTING CENTER – BARCELONA, SPAIN

VISITING POSTDOC

GRID COMPUTATIONAL CHEMISTRY – GRID-COMPCHEM – Marie-Curie Host Fellowship for the Transfer of Knowledge
EU ToK grant No. MTKD-CT-2005-029583 & HPC-Europa2 Scholarship

INSTITUTE OF ELECTRONIC STRUCTURE AND LASER OF THE FOUNDATION FOR RESEARCH AND TECHNOLOGY HELLAS – HERAKLION, CRETE, GREECE

RESEARCH COLLABORATOR – 2006 – 2010

GRID COMPUTATIONAL CHEMISTRY – GRID-COMPCHEM – Marie-Curie Host Fellowship for the Transfer of Knowledge
EU ToK grant No. MTKD-CT-2005-029583

EDUCATION AND TRAINING

30/09/1996 – 20/07/2000 Heraklion, Greece
BACHELOR DEGREE IN CHEMISTRY Department of Chemistry, University of Crete

Grants:
Entry Exam IKY Award - Scholarship (1996), (2) 1st, 2nd, 3d and 4th year IKY Scholarship for Excellence (1996-2000), (3) 3d year Award for Excellence (Municipality of Heraklion), (4) Award of Excellence in Graduation, University of Crete – Department of Chemistry (2000).

Address Voutes, 715 00, Heraklion, Greece | **Field of study** Chemistry | **Final grade** 8.87/10

06/2000 – 07/2006 Heraklion, Greece
MASTER'S - PH.D DEGREES Department of Chemistry, University of Crete

Msc Title: "The mechanism of O-O cleavage in Cytochrome *c* Oxidase as reevealed by Density Functional Theory and *resonance* Raman".
Ph.D Title: "Bioenergetic Mechanisms of O_2 and NO by Density Functional Theory".

Courses: (a) Special Topics in Biochemistry, (b) Pharmaceutical Chemistry, (c) IR/Raman Spectroscopy for Biological Molecules, (d) Computational Environmental Chemistry, (e) Multidimensional NMR Spectroscopy, (f) Vibrational Spectroscopy

(1) ***Visiting Ph.D*** **Grant-in-Aid for Scientific research** (**Grant-in-Aid for Specially Promoted Research**) **FY2005**. **Okazaki Institute** for Integrative Bioscience, National Institutes of Natural Sciences Supercomputing Center, **Okazaki, Aichi /Japan** (2005).
(2) IKY Scholarship for entry to the Postgraduate Programme (2001-2002), (2) **Maria Manasaki** Scholarship (2001-2002, 2002-2003)
(3) Project title: **Dynamics and reactivity of enzymatic processes involving heme-copper aa3 oxidase from P. denitrificans: Spectroscopy and theoretical studies**
Financial entity: **Greek Ministry of Education - Pythagoras I (2006)**
(4) Project title: **Bioenergetic mechanisms of O_2 and NO as revealed by density functional theory**
Financial entity: **Greek Ministry of Education / E.U. Hrakleitos (2002-2005)**
(5) Project title: **Structural Analysis of nitric oxide reductrase (nor)**
Financial entity: **Greek Ministry of Education, General Secretariat for Scientific Research (2000-2001)**

Address Voutes, Hreaklion, 715 00, Heraklion, Greece | **Field of study** Computational Biophysical Chemistry |

Final grade 9.75/10

LANGUAGE SKILLS

Mother tongue(s): **GREEK**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C2			C2	C2
FRENCH	B1			B1	B1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

RESEARCH

CURRENT
OUTPUT

53 publications as articles in **peer-reviewed journals (46)**, **book chapters (6)** and **conference proceedings (1)**. First author in 22/52 and the **corresponding author in 23/53** publications, exerting strong independence (h-index Scopus 17, Google Scholar 22, i10-index 31). Publications in leading journals of biophysics, physical chemistry and biomolecular dynamics (i.e. J. Am. Chem. Soc. Proc. Natl. Acad. Sci USA, Biochim. Biophys. Acta, NPG Commun. Chemi, Sci. Rep., J. Phys. Chem. BC, Phys. Chem. Chem. Phys., Chem. Commun., J Biomol. Struct. and Dynamics). Reviewer duties for Nature Journals, ACS Physical Chemistry Journals, RSC Phys. Chem. Chem. Phys., RSC Advances, Springer J. Molecular Modeling (**more than 270 Reviews for Journals, Web of Science – publons**, **Outstanding Reviewer for Phys. Chem. Chem. Physics 2024;** Phys. Chem. Chem. Phys. 2025, 27, 12111-12111). Reviewer for proposals to High Performance Computing (HPC) facilities (CyTera and Cyclone at the Cyprus Institute, GRNET ARIS HPC - the National Infrastructures for Research and Technology, CSCS-Swiss National Supercomputing Centre, Institute for Advanced Simulation (IAS), Jülich Supercomputing Centre (JSC), Gauss Centre for Supercomputing (GCS) and the John von Neumann Institute for Computing (NIC)). Evaluator for the Biotechnology and Biological Sciences Research Council (BBSRC) and Czech Science Foundation. **44 participations in International Conferences - Seminars**, including **13 invited lectures**. My research is featured in the PRACE DIGEST 2017, 2020 from Insight Publishers.

CURRENT

The Lab of Biomolecular Dynamics and Engineering

My independent research focuses on the biophysics of large biological molecules involved in processes related to life sciences (Biology, Biomolecular Engineering): **Heme proteins, Photosystem II Light Harvesting Complexes, SARS-CoV-2 proteins, Intrinsically Disordered Proteins and Condensates, Protein Thermostability, the CRISPR-Cas and Fanzor systems**
In the lab we employ elaborate computational techniques based on the Molecular Dynamics (MD) method (accelarated MD, metadynamics in the multiwalkers variant, or the parallel tempering metadynamics at the well-tempered ensemble variant), in combination with ab-initio Density Functional Theory (DFT) Methods. The setup of the models and the analysis of the results is based on bioinformatics tools (protein-protein docking algorithms, sequence and structural alignments, Markov State Modeling). We have benefitted from various projects in High Performance Computing (HPC) facilities awarded within the EuroHPC JU (https://www.eurohpc-ju.europa.eu), PRACE/ DECI (https://prace-ri.eu/) schemes (Joliot Curie - Irene ROME TGCC in Bruyères-le-Châtel, Salomon iT4i Czech Republic, SuperMUC-NG LRZ Munich, HLRS Stuttgart, MareNostrum Barcelona Supercomputing Center). My dual insight in combining both computational and experimental biochemistry, biophysics and biological chemistry makes me a competent researcher in the field.

PUBLICATIONS

01. Conformational plasticity enables functional switching in diatom lightharvesting complexes

Sousani TI, Zender B, Maity S, Kleinekathöfer U, and **Daskalakis V*** (2025) ***Commun Chem*** 8, 392 https://doi.org/10.1038/s42004-025-01774-x

02. An Unexpected Water Channel in the Light-Harvesting Complex of a Diatom: Implications for the Switch between Light Harvesting and Photoprotection

Daskalakis V*, Maity S and Kleinekathöfer U (**2025**) ***ACS Phys. Chem Au*** 5, 1, 47–61. *doi:* 10.1021/acsphyschemau.4c00069 (***January 2025 Journal Cover***)

03. Hydrophobic mismatch in the thylakoid membrane regulates photosynthetic light harvesting

Wilson S, Clarke C, Carbajal MA, Buccafusca R, Fleck R, **Daskalakis V**, and Ruban, A***** (**2024**) ***J. Am. Chem. Soc.*** 146, 21, 14905–14914**.** DOI: 10.1021/jacs.4c05220

04. Acclimation mechanism of microalgal photosynthetic apparatus under low atmospheric pressures – New astrobiological perspectives in a Mars like atmosphere

Gritsi CS, Sarmas E, **Daskalakis V** and Kotzabasis K* (2024) ***Functional Plant Biology*** 51, FP24058, doi:10.1071/FP24058

05. Electric Field Susceptibility of Chlorophyll c Leads to Unexpected Excitation Dynamics in the Major Light-Harvesting Complex of Diatoms

Maity S, **Daskalakis V**, Jansen LCT, and Kleinekathöfer U* (**2024**) ***J. Phys. Chem. Lett.*** 15, 9, 2499–2510

06. The synergy between the PscC subunits for electron transfer to the P840 special pair in Chlorobaculum tepidum

Daskalakis V, Lyratzakis A, Xie H, and Tsiotis G* (**2024**) ***Photosynth Res*** 160, 87–96. doi: 10.1007/s11120-024-01093-7

07. Engineering salt-tolerant Cas12f1 variants for gene-editing applications

Daskalakis, V* and Papapetros, S (**2023**) **J. Biomolecular Struct. and Dynamics**, doi: 10.1080/07391102.2023.2240418

08. Recognition motifs for Importin 4 [(L)PPRS(G/P)P] and Importin 5 [KP(K/Y)LV] bind-ing, identified by bio-informatic simulation and experimental in vitro validation

Panagiotopoulos AA, Kalyvianaki K, Tsodoulou PK, Darivianaki MN, Dellis D, Notas G, **Daskalakis V**, Theodoropoulos PA, Panagiotidis CA, Castanas E, Kampa M* (**2022**) **Comp. Struct. Biotechnol. J.** doi: 10.1016/j.csbj.2022.10.015

09. Deciphering the QR code of the CRISPR-Cas9 system: Synergy between Gln768 (Q) and Arg976 (R)

Daskalakis V* (**2022**) ***Journal of Physical Chemistry Au***. doi: 10.1021/acsphyschemau.2c00041

10. Trivial Excitation Energy Transfer to Carotenoids is an Unlikely Mechanism for Non-Photochemical Quenching in LHCII

Gray C, Wei T, Polívka T, **Daskalakis V**, and Duffy CDP* (**2022**) ***Front. Plant Sci.*** 12: 797373.

11. Natural polyphenols inhibit the dimerization of the SARS-CoV-2 main protease: the case of fortunellin and its structural analogs

Panagiotopoulos AA, Karakasiliotis I, Kotzampasi D-M, Dimitriou M, Sourvinos G, Kampa M, Pirintsos S, Castanas E* and **Daskalakis V*** (**2021**) **Molecules** (**MDPI**), *26, 6068*

12. Robust Strategy for Photoprotection in the Light-Harvesting Antenna of Diatoms: A Molecular Dynamics Study

Chrysafoudi A, Maity S, Kleinekathöfer U and **Daskalakis V*** (**2021**) **J. Phys. Chem. Lett.** 12, 9626−9633

13. Time-Dependent Atomistic Simulations of the CP29 Light-Harvesting Complex

Maity S, Sarngadharan P, **Daskalakis V**, and Kleinekathöfer U* (**2021**), ***J. Chem. Phys.*** 155, 055103

14. Hydrogen gas as a central on-off functional switch of reversible metabolic arrest – New perspectives for biotechnological applications

Zerveas S, Kydonakis E, Mente M-S, **Daskalakis V**, and Kotzabasis K (**2021**) **J. Biotechnology**, *335: 9 - 18*

15. p-cymene impairs SARS-CoV- 2 and Influenza A (H1N1) viral replication: In silico predicted interaction with SARS-CoV- 2 nucleocapsid protein and H1N1 nucleoprotein

Panagiotopoulos A, Tseliou M, Karakasiliotis I, Kotzampasi D-M, **Daskalakis V**, Kesesidis N, Notas G, Lionis C, Kampa M, Pirintsos S, Sourvinos G, Castanas E. (**2021**) ***Pharmacol Res Perspect.*** 9:e00798

16. Multiscale QM/MM Molecular Dynamics Simulations of the Trimeric Major Light-Harvesting Complex II

Maity S, **Daskalakis V**, Elstner M and Kleinekathöfer U* (**2021**) ***Phys. Chem. Chem. Phys***, 23, 7407 – 7417

17. The conformational phase space of the photoprotective switch in the major Light Harvesting Complex II

Daskalakis V*, Papadatos S, Stergiannakos, **(2020) Chem. Commun.** 56, 11215 – 11218

18. Structure and Dynamics of a Thermostable Alcohol Dehydrogenase from the Antarctic Psychrophile Moraxella sp. TAE123

Petratos K*, Gessmann R, **Daskalakis V**, Papadovasilaki M, Papanikolau Y, Tsigos I , and Bouriotis V **(2020) ACS Omega**, 5, 24, 14523–14534

19. Structural Basis for Allosteric Regulation in the Major Antenna Trimer of Photosystem II

Daskalakis V*, Maity S, Hart CL, Stergiannakos T, Duffy CDP, and Kleinekathöfer U **(2019)** ***J. Phys. Chem. B,*** *123*, 45, 9609-9615

20. Fine tuning of the photosystem II major antenna mobility within the thylakoid membrane of higher plants

Daskalakis V*, Papadatos S, Kleinekathoefer, U (**2019**) ***Biochim. Biophys. Acta – Biomembranes*****,** *1861*, 183059

21. On a Chlorophyll-Carotenoid Coupling in LHCII

Maity S, Gelessus A, **Daskalakis V**, Kleinekathoefer, U* (**2019**) ***Chem. Phys.*** *526,* 110439

22. Protein-Protein Interactions within Photosystem II under Photoprotection: The Synergy between CP29 Minor Antenna, Subunit S (PsbS) and Zeaxanthin at all-atom resolution

Daskalakis V* (**2018**) ***Phys. Chem. Chem. Phys.*** *20*, 11843 – 11855

23. The Photosystem II Subunit S under Stress

Daskalakis V*, and Papadatos S (**2017**) ***Biophys. J. (Cell)*** *113 (11)*, 2364-2372.

24. A pathway for protective quenching in antenna proteins of Photosystem II

Papadatos S, Charalambous C A, and **Daskalakis V*** (**2017**) ***Scientific Reports (NPG)*** *7,* 2523. doi: 10.1038/s41598-017-02892-w.

25. Detection of Maillard reaction products by a coupled HPLC-Fraction collector technique and FTIR characterization of Cu(II)-complexation with the isolated species

Ioannou A, **Daskalakis V**, and Varotsis C* (**2017**) ***J. Mol. Struct.*** *1141*, 634–642.

26. Coupling of helix E-F motion with the O-nitrito and 2-nitrovinyl coordination in myoglobin

Ioannou A, Lambrou A, **Daskalakis V*** and Pinakoulaki E* (**2017**) ***Biophys. Chem.*** *221,* 10-16.

27. Nitrite coordination in myoglobin

Ioannou A, Lambrou A, **Daskalakis V** and Pinakoulaki E* (**2017***) **J. Inorg. Biochemistry (JIB)**, 166, 49-54.*

28. Energizing the Light Harvesting Antenna: Insight from CP29

Ioannidis NE, Papadatos S, and **Daskalakis V*** (**2016**) ***BBA – Bioenergetics***, *1857 (10), 1643-1650.*

29. Correlation Between Surface Tension and the Bulk Dynamics in Salty Atmospheric Aquatic Droplets

Salameh A, Vorka, F, and **Daskalakis V* (2016)** ***J. Phys. Chem. C***, *120 (21), 11508-11518*

30. Structure and properties of the catalytic site of nitric oxide reductase at ambient temperature

Daskalakis V, Ohta T, Kitagawa T, Varotsis C* **(2015)** ***Biochim. Biophys. Acta – Bioenergetics***, 1847(10), 1240–1244.

31. Surface-Active Organic Matter induces salt morphology transitions during new atmospheric particle formation and growth

Daskalakis V*, Charalambous F, Demetriou DC, Georgiou AG **(2015)** ***RSC Adv.***, 5, 63240–63251.

32. Effects of Surface Activity on Carbon Dioxide Nucleation in Atmospheric Wet Aerosols: A Molecular Dynamics Study

Daskalakis V*, Charalambous F, Panagiotou F, Nearchou I **(2014)** ***Phys. Chem. Chem. Phys.***, 16: 23723-23734.

33. Hexagonal Ice Stability and Growth in the presence of Glyoxal and Secondary Organic Aerosols

Daskalakis V*, Hadjicharalambous M **(2014)** ***Phys. Chem. Chem. Phys.*** 16(33): 17799-17810.

34. The protein effect in the structure of two ferryl-oxo intermediates at the same oxidation level in the heme-copper binuclear center of cytochrome c oxidase

Pinakoulaki E, **Daskalakis V**, Ohta T, Richter O M, Budiman K, Kitagawa T, Ludwig B, Varotsis C* **(2013)** ***J. Biol. Chem.*** 288(28): 20261-20266.

35. Exploring the Topography of Free Energy Surfaces and Kinetics of Cytochrome c Oxidases interacting with small ligands

Porrini M, **Daskalakis V**, Farantos SC* **(2012)** ***RSC Adv.*** 2: 5828 - 5836.

36. Non-Linear Vibrational Modes in Biomolecules: a periodic orbits description

Kampanarakis A, Farantos SC*, **Daskalakis V** and Varotsis C **(2012)** ***Chem. Phys. Elsevier***, 399: 258–263.

37. The origin of the FeIV=O intermediates in cytochrome aa3 oxidase

Pinakoulaki E, **Daskalakis V** and Varotsis C* **(2012)** ***BBA Bioenergetics***, 1817: 552-557.

38. Regulation of Electron and Proton Transfer by the Protein Matrix of Cytochrome c Oxidase

Daskalakis V, Farantos SC, Guallar V, Varotsis C* (**2011**) ***J. Phys. Chem. B***, 115(13): 3648-3655

39. Vibrational Resonances and CuB displacement controlled by proton motion in Cytochrome c Oxidase

Daskalakis V*, Farantos SC, Guallar V, Varotsis C (**2010**) ***J. Phys. Chem. B***, 114(2): 1136-1143

40. Binding and Docking Interactions of NO, CO and O2 in Heme Proteins as Probed by Density Functional Theory

Review for the Special Issue on “Application of Density Functional Theory in Chemical Reactions”
Daskalakis V, Varotsis C* (**2009**) ***Int. J. Mol. Sci.,*** 10: 4137-4156

41. Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: The Role of Ring-D Propionate

Porrini M*, **Daskalakis V**, Farantos SC, Varotsis C *(***2009**) ***J. Phys. Chem. B***, 113(35): 12129-12135

42. Assigning vibrational spectra of ferryl-oxo intermediates of cytochrome c oxidase by periodic orbits and Molecular Dynamics

Daskalakis V, Farantos SC*, Varotsis C *(***2008***) **J. Am. Chem. Soc*** 130(37): 12385-12393

43. Probing the environment of CuB in heme-copper oxidases

Daskalakis V, Pinakoulaki E, Stavrakis S, Varotsis C* (**2007**) ***J. Phys. Chem. B*** 111: 10502-10509

44. Two ligand binding sites in the O2-sensing signal transducer HemAT: Implications for ligand Recognition/ Discrimination and signaling

Pinakoulaki E, Yoshimura H, **Daskalakis V**, Yoshioka S, Aono S, Varotsis C* (**2006**) ***Proc. Natl. Acad. Sci. USA*** 103: 14796-14801

45. Structural dynamics of Heme-copper oxidases and Nitric oxide reductases: Time-Resolved step-scan FTIR and Time-resolved Resonance Raman studies

Pinakoulaki E, Koutsoupakis C, Stavrakis S, Marialena A, Papadopoulos G, **Daskalakis V**, Varotsis C* (**2005**) ***J. Raman Spec.*** 36: 337-349

46. Time-resolved step-scan Fourier transform infrared investigation of heme-copper oxidases: implications for O2 input and H2O/H+ output channels

Koutsoupakis C, Pinakoulaki E, Stavrakis S, **Daskalakis V**, Varotsis C* (**2004**) ***Bioch. Biophys. Acta*** 1655: 347-352

REVIEW ARTICLES/ BOOK CHAPTERS----------

47. From Traditional Ethnopharmacology to Modern Natural Drug Discovery: A Methodology Discussion and Specific Examples

Book Chapter-Perspective: Pirintsos S, Panagiotopoulos A, Bariotakis M, **Daskalakis V**, Lionis C, Sourvinos G, Karakasiliotis I, Kampa M, and Castanas E. (**2022**) ***MDPI Molecules***, 27(13), 4060.

48. A perspective on the Major Light Harvesting Complex Dynamics Under the Effect of pH, Salts and the Photoprotective PsbS Protein

Book Chapter-Perspective: Navakoudis E, Stergiannakos T, and **Daskalakis V*** (**2022**) *Quantum and classical computational methods in photosynthesis: from the atom to the mesoscale* in ***Photosynthesis Research,*** doi: 10.3390/ molecules27134060

49. Atmospheric Ice Nucleation by Glassy Organic Compounds: A Review

Book Chapter-Review: Salameh A, and **Daskalakis V*** (**2017**), **Chem. Comp. J** 1(1): 13-23

50. Probing the Action of Cytochrome c Oxidase (2014) The Structural Basis of Biological Energy Generation

Book Chapter-Review: Daskalakis V, Varotsis C* **Advances in Photosynthesis and Respiration**, 39 (10): SBN 978-94-017-8742-0

51. Tuning heme functionality: the cases of Cytochrome c Oxidase and Myoglobin Oxidation

Book Chapter-Review: Daskalakis V*, Farantos S C, Varotsis C **(2012), LNCS – Springer-Verlag Berlin, Heidelberg**, p. 304-315. ISBN: 978-3-642-31124-6

52. Grid Computing Multiple Shooting Algorithms for Extended Phase Space Sampling and Long Time Propagation in Molecular Dynamics

Book Chapter-Review: Daskalakis V, Giatromanolakis M, Porrini M, Farantos, SC* and Gervasi O ***Computer Physics,*** *Chapter 4 pp. 1-18,* ***2011*** *© Nova Science Publishers,* Inc. *Editors: B. S. Doherty, A. N. Molloy.* ISBN 978-1-61324-790-7

53. Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach

Conference Proceedings: Daskalakis V*, Farantos SC, Varotsis C (**2007**) ***AIP Computation in Modern Science and Engineering, Proc.*** 963(2): 31-34

CONFERENCES AND SEMINARS

2023 – 2025

Conferences - Seminars - Workshops

1. Sousani TI, Zender B, Maity S, Kleinekathöfer U and **Daskalakis V*** "Intrinsic Conformational Plasticity Fine-Tunes Light Harvesting in Diatoms". Extended Hanseatic meeting on Exciton Dynamics and Spectroscopy 2025, Vilnius, Lithouania, September 29 - October 4, 2025 (invited talk).

2. Karvounis IG, Tsiavou V, and **Daskalakis V*** "Molecular Dynamics of RNA-Guided Endonucleases: Comparative Insights into Cas12 and Eukaryotic Fanzor Systems". The 5th International Symposium on Frontiers in Molecular Science, Kyoto, Japan, August 26-29, 2025.

3. Daskalakis V* "Baila Morena: The Choreography of Proteins Under a Computational Microscope". ICFO FRONTIERS RESEARCH SCHOOL: Physics for Biology and Medicine, Barcelona, Spain, July 7-11 2025 (invited talk).

4. Theofani-Iosifina Sousani and **Daskalakis V*** "Light-induced transfer of a proton in the light-harvesting complexes of diatoms". ACS Spring 2025 Meeting & Expo, San Diego, CA, USA, March 23-27.

5. Daskalakis V*, Maity S, Kleinekathöfer U. "Diatoms under Computational Sunlight". Second European Congress on Photosynthesis Research (ePS2 2024), Padova, Italy, 25-28 June 2024.

6. Karampa P, Makryniotis K, Nikolaivits E, **Daskalakis V**, Topakas E, Dimarogona M*. "Investigation of Structural Determinants of Plastic Degrading Enzymes via x-ray Crystallography and Molecular Docking". 14th Hellenic Scientific Conference in Chemical Engineering, Thessaloniki, Greece, 29-31 May 2024.

7. Daskalakis V. "CRISPR-Cas proteins: Engineering of "silver-bullets" in the arsenal of gene editing". International Society of Quantum Biology and Pharmacology (ISQBP2024) President's Meeting, Athens, Greece, 19-23 May 2024.

8. Daskalakis V. "*Biomolecular Simulations: From Dynamics to Engineering*". Seminar at the Foundation for Research and Technology Hellas / Institute of Chemical Engineering Sciences (FORTH/ICE-HT), 17 April 2024 (*invited talk*)

9. Daskalakis V. "*Biomolecular Engineering: Structures and Dynamics*". Seminar at the Department of Physics, Constructor University, Bremen, Germany, 27 April 2023 (*invited talk*)

10. Daskalakis V. "*Biomolecular Engineering: Structures and Dynamics*". Seminar at the Institute of Marine Biology, Biotechnology and Aquaculture (IMBBC), Hellenic Centre for Marine Research (HCMR), Heraklion, Greece, 03 May 2023 (*invited talk*)

11. Daskalakis V. "*Biomolecular Engineering: Structures and Dynamics*". Seminar Department of Chemistry, *Aristotle University* of Thessaloniki, Greece, 15 May 2023 (*invited talk*)

2020 – 2022

Conferences - Seminars - Workshops

1. Daskalakis V.*"CRISPR-Cas9: From Biomolecular Engineering to Dynamics*". Joint Seminar Series in Biotechnology, Biosciences, and Biomedical Research of the University of Ioannina (School of Medicine), co-organized by IIPPS - Mol Cell Biol Biotechnol, URCI - Institute of Biosciences, IMBB-FORTH, Biomedical Research Dept. (BRI-FORTH), 16 December 2022 (online, *invited talk*)

2. Daskalakis V. *"From Rigid Crystal Structures to Conformational Sampling: A tale of two Light Harvesting Complexes*". Virtual international conference Computational methods in photosynthesis: From atoms to the mesoscale, from theory to experiment (ComPhot2021), November 8-11, 2021 (online, *invited talk*)

3. Daskalakis V. *"From Rigid Crystal Structures to Conformational Sampling: A tale of two Light Harvesting Complexes*". Virtual HPC-Europa3 TAM Meeting, November 3-4, 2021 (online talk)

4. Daskalakis V. "The mechanics of photoprotection in the major antenna of Photosystem II: let there be light...", SuperMUC-NG Status and Results Workshop, 8-10 June 2021 (online, invited talk).

5. Daskalakis V. "High Performance Computing in Structural Biology", CaSToRC - The Cyprus Institute, 19 January 2021 (online, *invited talk*)

6. Daskalakis V. "Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution", EuroHPC Summit Week, 22-26 March 2021 (online, *invited talk*)

2014 – 2020
Conferences - Seminars - Workshops

7. Daskalakis V. COVID-19 pandemic – What have we learned and what does the future hold? Online Seminar, The Cyprus Institute, December 5 2020 (*invited talk*)

8. Daskalakis V., Stergiannakos T., Papadatos, S. **The Synergy between LHCII and PsbS under Photoprotection**, Biophysics of Photosynthesis 2019, Accademia dei Lincei, Rome Italy, October 2-4, 2019

9. Daskalakis V., Stergiannakos T., Papadatos, S. **The Photosynthetic Apparatus under Stress by Molecular Simulations**, Photosynthesis Gordon Research Conference, Grand Summit Hotel at Sunday River in Newry, ME United States, July 21-16, 2019 *(by invitation only).*

10. Daskalakis V. Lecture, **Fine Tuning of the Photosynthetic Apparatus**, Department of Materials Science and Technology, Heraklion, Greece, 20 May 2019 *(invited talk).*

11. Daskalakis V. Lecture, **The Photosynthetic Apparatus under Stress by Molecular Simulations**, National Hellenic Research Foundation, Athens, Greece, 17 December 2018 *(invited talk).*

12. Daskalakis V. Molife Research Seminar, **Triggering Photoprotection in Photosystem II Light Harvesting Complexes by Molecular Simulations**, Bremen, Germany GmbH, 25 September 2018 *(invited talk).*

13. Daskalakis V. 62 nd Annual Meeting Biophysical Society, **S(T)IMULATING THE INTERPLAY BETWEEN PHOTOSYSTEM II PROTEINS AND THE XANTHOPHYLL CYCLE IN PHOTOPROTECTION**, San Francisco, USA, 17-21 February 2018

14. Daskalakis V. 3d EMN Meeting on Computation and Theory – Molecular Dynamics and Its Applications, **The effect of proton and potential gradients on integral membrane proteins: Insights from Molecular Dynamics simulations**, Dubai UAE, 6-10 November 2017 (Invited Talk)

15. Daskalakis V, Papadatos S**.** 42nd FEBS Congress (from molecules to cells and back) – **The Photosystem II Subunit S Dynamics under Stress**, Jerusalem Israel, 10-14 September 2017 (Poster).

16. Daskalakis V, Salameh A, AGU 2016 Fall Meeting – ***Correlation Between Surface Tension and the Bulk Dynamics in Salty Atmospheric Aquatic Droplets, San Francisco USA, 12-16 December 2016 (Poster).***

17. Daskalakis V, Department of Chemistry University of Crete Seminars, ***Oxygen Evolution and Reduction: Common Principles***, *Heraklion-Crete, Greece, 25 November 2017 (invited talk).*

18. Daskalakis V, Ioannidis NE, Papadatos S**.** 79th Harden Conference – Oxygen Evolution and Reduction – Common Principles**: Tuning of a conformational change in CP29 from spinach: from Light Harvesting to Photoprotection**, Innsbruck Austria, 16-20 April 2016 (Poster+Talk).

19. Daskalakis V and Pinakoulaki E. New Biological Frontiers Illuminated by Molecular Sensors and Actuators meeting being held in Taipei, Taiwan, June 28 – July 1, 2015. Abstract titled "Globin Nitrito Heme Fe-O-N=O/ 2-Nitrovinyl Species: Impications for Myoglobin Helices Dynamics", fixed-participants meeting.

20. Organizational Committee "12th Greece-Cyprus Conference on Chemistry 2015", 8-10 May 2015, Thessaloniki Greece

2009 – 2014

Conferences - Seminars - Workshops

21. Daskalakis V, Hadjicharalambous M, Charalambous F ***Ice 1_h crystal stability and growth in the presence of glyoxal Secondary Organic Aerosol and Carbon Dioxide***. 13th Quadrennial IGACGP Symposium 13th IGAC Science Conference on Atmospheric Chemistry (IGACGP, IGAC 2014), Brazil, Natal, 22-26 September, 2014.

22. Daskalakis V, Hadjicharalambous M ***Probing the Effects of Atmospheric Pollutants on Ice Nucleation***. International Conference on Scientific Computing 2013 (CSC 2013), Paphos, Cyprus, 3 - 6 December 2013. (Invited talk).

23. Daskalakis V, Varotsis C **The structure of the Hyponitrite in Nitric Oxide Reductase (NOR)**. Biophysical Society (BPS) 57th Annual Meeting in Philadelphia, Pennsylvania, February 2-6, 2013.

24. Daskalakis V, ASEMUNDUS Networking seminar in Korea. Erasmus Mundus programme to enhance quality in higher education through scholarships and academic cooperation between Europe and the rest of the world. Seoul, Korea, May 15-16, 2012.

25. Daskalakis V, Farantos S C, Varotsis C ***Tuning heme functionality: the cases of Cytochrome c Oxidase and Myoglobin Oxidation***, **12th International Conference on Computational Science and Applications** (**ICCSA 2012**), **June 18-21, Salvador de Bahia, Brazil, 2012.** *(Best paper Award)*

26. Daskalakis V, Varotsis C ***Probing the effect of the proximal and distal to the heme a_3 environments in the Cytochrome c Oxidase dioxygen reaction***, 15th International Conference on Biological Chemistry (ICBIC15), 7-12 August, Vancouver, Canada, 2011.

27. CD-ADAPCO, STAR-CCM+ Training School, 10-12 May 2011, London, UK.

28. Daskalakis V, Farantos S C, Guallar V, Varotsis C ***QM/MM Calculations on Cytochrome c Oxidase: Probing of electron and proton pump coupling***, TAM 2010 MEETING, Helsinki 15-17 June 2010.

2001 – 2010

Conferences - Seminars - Workshops

29. Expanding the Frontiers of Molecular Dynamics Simulations in Biology, 23-25 November, Institu d' Estudis Catalans, Barcelona – Spain, 2009 (Joint BSC - IRB Barcelona Conference).

30. Aug. 31 – Sept. 5 2009: Summer School on Simulation Approaches to Problems in Molecular and Cellurar Biology, Miramar Palace, San Sebastian, Spain. **Cecam** (Centre Europeen de Calcul Atomique et Moleculaire), *under* **Psi-K** *scholarship*.

31. Daskalakis V, Farantos S C, Guallar V, Varotsis C ***Towards the Understanding of His411-Fe^{IV}=O Spectroscopic Properties in Ferryl Intermediate of Cytochrome c Oxidase + O_2 Reaction: A Theoretical QM/MM, MD Approach***, 14th International Conference on Biological Inorganic Chemistry (ICBIC14), 25-30 July, Nagoya, Japan, 2009. ***SBIC (The Society of Biological Inorganic Chemistry)*** *Poster Award for outstanding contribution***.**

32. Porrini M**, Daskalakis V**, Farantos SC, Varotsis C ***Heme cavity dynamics of photodissociated CO from ba_3-cytochrome c oxidase: The role of ring-D propionate***, 10th Congress in Chemistry Greece – Cyprus, 2-4 July Heraklion, Greece, 2009.

33. a. Daskalakis V, Farantos C S, Varotsis C **Assigning Vibrational Spectra of Ferryl-Oxo Intermediates of Cytochrome *c* Oxidase by Periodic Orbits and Molecular Dynamics,**

b. Daskalakis V, Varotis C **Cytochrome *c* Oxidase + O_2 reaction intermediates as probed by Density Functional Theory: The Proximal and Distal to heme a_3 effects,**

c. Daskalakis V, Varotsis C **Theoretical Studies of Metal-NO*x* species, isolated and in aqueous solutions: Raman bands,** 10th Congress in Chemistry Greece – Cyprus, 2-4 July Heraklion, Greece, 2009.

34. 15-18 Sept. 2008: **Cost Training School On Molecular And Material Science Grid Applications** - Trieste, Italy.

35. Gervasi O, Farantos S C, **Daskalakis V**, Giatromanolakis M ***The Study of cytochrome c Oxidase on the EGEE Grid***, *3d EGEE User Forum*, *Clemont-Ferrand, France, 2008.*

36. Daskalakis V, Giatromanolakis M, Farantos SC, Gerbasi O ***EGEE: Applications in Classical and Quantum Molecular Dynamics,*** *First Hellas Grid User Forum*, *Athens, Greece*, 2007*.*

37. Daskalakis V, Farantos S, Varotsis C ***Protein dynamics and spectroscopy for ferryl intermediate of Cytochrome c Oxidase: A molecular dynamics approach*****,*** International Conference of Computational Methods in Sciences and Engineering (**ICCMSE 2007**), *Corfu, Greece,* 2007. *(Award for Best Presentation, by the Organizing Committee of ICCMSE)*
Publication: ***Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach***, ***AIP Computation in Modern Science and Engineering, Proc.*** 963(2): 31-34 (**2007**).

38. Pinakoulaki E, Ohta T, **Daskalakis V**, Aggelaki M, Kitagawa T, Ludwig B, Varotsis C **, ISBC2006**, Konan Fiber, Fiber, Konan University, Japan, 2006*.*

39. Daskalakis V, Frudakis G, Varotsis C ***DFT Study of endoperoxides and their intermediates in Fe(II) cleavage of the endoperoxy bridge,*** 19th National Conference in Chemistry*,* Heraklion, Crete, Greece*,* 2002.

NETWORKS AND MEMBERSHIPS

INTERNATIONAL COLLABORATIONS (OLD & CURRENT)

Heme proteins
Prof. Varotsis Constantinos, Dept. Chemical Engineering, Cyprus University of Technology, Cyprus
Prof. Farantos Stavros, Dept. of Chemistry, University of Crete & Foundation for Research and Technology-Hellas
Prof. Teizo Kitagawa, Specially Appointed Professor; Graduate School of Life Science, University of Hyogo
Prof. Guallar Victor, ICREA Research Professor at Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS). Life & Medical Sciences.

Photosynthesis
Prof. Alexander Ruban, School of Biological and Chemical Sciences, Queen Mary, University of London
Prof. Ulrich Kleinekathöfer, Computational Physics and Biophysics Group, Jacobs University Bremen gGmbH, Department of Physics & Earth Sciences Focus Area Health
Dr. Christopher Duffy, Cellular and Molecular Biology, School of Biological and Chemical Sciences, Queen Mary, University of London
Prof. Kentaro Ifuku, University of Kyoto, Japan.

Protein Thermostability - Intinsically Disordered Proteins
Dr. Kyriacos Petratos, Principal Researcher, Laboratory of Crytallography, Institute of Molecular Biology and Biotechnology, Foundation for Research and Technology Hellas (FORTH).
Prof. Kotzabasis Kiriakos, Dept. Biology, University of Crete, Greece
Assoc. Prof. Panagiotis Nikolaou Moschou, Dept. Biology, University of Crete, Greece, Foundation for Research and Technology - Hellas, Swedish University of Agricultural Sciences

SARS-CoV-2 Targets
Prof. Elias Castanas, School of Medicine, University of Crete
Prof. Stergios Pirintsos, Dept. Biology, University of Crete, Greece

Protein Transporters
Prof. Stathis Frillingos, School of Medicine, University of Ioannina

MANAGEMENT AND LEADERSHIP SKILLS

Mentoring

University of Patras (2023 - present)

Doctoral Theses/ Candidates (Ph.D degree):
Current (3): Theofani Iosifina Sousani, Boutheina Zender, Ilias Karvounis

Research Collaborators:
Current (1): Panos Koukos (post-doc)
Former (2): Ariadni Konstantopoulou (post-doc), Konstantinos Chatzikyriakos(research - associate)

Undergraduate Diploma Theses (Engineering Diploma)
Current (6): Anastasia Iakovou, Minasian Azat, Natalia Chroni, Kaliopi Karantzi, Natalia Emmanouilidi, Andreas Gousgounellis
Completed (3): Tsikli Theoni, Tsiavou Valentina, Nitas Panagiotis

Participation in Examiner's Board for doctoral defences:

1. Sotiris Zerveas (University of Crete, Dept. Biology)
2. Maria Polychronaki (University of Crete, Dept. Chemistry)
3. Christos Kosinas (University of Patras, Dept. Chem. Eng.)
4. Alexandros Lyratzakis (University of Crete, Dept. Chemistry)
5. Danai Maria Kotzampasi (University of Crete, Dept. Biology)
6. Panagiota Siachouli (Foundation for Research and Technology - Hellas, FORTH)
7. Vasiliki K. Valianti (University of Cyprus, Dept. of Chemistry)

Cyprus University of Technology (2010-2023)

Undergraduate Diploma Theses (Bachelors' degree)
Completed (9): Charalambous Fevronia, Ioannou Neofyta, Panagiotou Fostira, Nearchou Irene, Demetriou D Constantinos, Georgiou A Georgia, Eleftheriou Antonis, Vorka Flora, Charalambous Andreas, Palazis K. Andreas, Katsoni Panagiota

Postgraduate Diploma Theses (Master's degree)
Completed (5): Charalambous Fevronia, Ioannou Neofyta, Papadatos Sotirios, Anthi Chrisafoudi (in collaboration w/ Dept. Biology, University of Crete), Danai Maria Kotzampasi (in collaboration w/ School of Medicine, University of Crete and Institute of Computer Science, Foundation for Research and Technology)

Doctoral Theses/ Candidates (Ph.D degree):
Completed (1): Salameh Anastasia

ACADEMIC & ADMINISTRATIVE DUTIES

01/09/2023 – CURRENT
University of Patras

1. Associate Editor, Frontiers in Chemistry, Theoretical and Computational Chemistry section
2. Premium Member of the American Chemical Society (2024-2025)
3. Member/ Committe of Postgraduate studies in the Department of Chemical Engineering, University of Patras (2024-2025)
4. Organization of seminars for the selection of undergraduate Diploma Thesis (2024-2025)
5. Member/ Committe of the joint programme in Chemical Engineering with Liaoning University of Technology (LUT).

01/12/2010 – 31/08/2023
Cyprus University of Technology

1. Member of the General Assembly of the Faculty of Geotechnical Sciences and Environmental Management (2023)
2. The Senatorial Committee of Information Systems and Technology (IST) (2012-2018)
(a) Reviews on the annual budgetary submissions from IST
(b) IdM (IAM) Project Committee for the implementation of the "Identity Access Management" scheme into the Cyprus University of Technology Information Systems & Technology (IST)
(c) Microsoft Software for Students Project Committee (IST)
(d) Committee for the Internet User Access Rights and Policies for Cyprus University of Technology
3. The Departmental Postgraduate (2011-2023) & Undergraduate Committees (2017-2023)
4. The Departmental Committee on Quality Assurance (2011-2023)
5. The Ad hoc ECTS label Committee of the Cyprus University of Technology (2014)
6. The Ad hoc committee for the Open University (2016-2023)
7. The committee of the Pancyprian Examinations for admission to Higher Education Institutions of Cyprus and Greece (2014)
8. Member of the election committee for the University Academic Board Members (2012)
9. RAC Allocation Committee for Computational time on Cyclone (The Cyprus Institute)

TEACHING DUTIES

Independent teaching

University of Patras, Dept. Chemical Engineering:
undergraduate courses (1) CHM-163 Computer Lab (Winter Semesters 2023-2025), (2) CHM-363 Introduction to Programming - Theory & Lab (Winter Semesters 2023-2025)
University of Patras, School of Medicine:
postgraduate course (1) Research Methodology in BioSciences BIE - Simulations of Biomolecular Interactions (2023-2024)
University of Ioannina, School of Medicine:

postgraduate course (1) Functional analysis of genes: from the design to the living system - Biomolecular Simulations & Drug design (2024-2025)
University of Crete, Department of Biology:
«Photosynthesis: The Photosynthetic apparatus under the microscope of Molecular Dynamics», in postgraduate program «Molecular and Applied Plant Biology – Green Biotechnology» (Autumn/ Spring Semesters 2019-2025)
University of Crete, School of Medicine:
«Under the Microscope of Molecular Dynamics», in postgraduate program «Bioinformatics» (Autumn Semester 2021)

Cyprus University of Technology Postgraduate:
(1) Computational Environmental Chemistry, Biochemistry and Biology (Spring Semesters 2012-2017), (2) Special Topics in Environmental Bioscience (Autumn Semester 2014)
Cyprus University of Technology Ungerdraduate:
(3) Environmental Computational Modeling & Introduction to MATLAB (Spring Semesters 2011-2020) (4) Dispersion Modeling (Autumn Semesters 2011-2020), (5) Environmental Physics (Autumn Semester 2011), (6) Principles of Thermodynamics & Chemical Kinetics (Spring Semesters 2011-2012), (7) Applied Thermodynamics II, (Spring semesters 2020-2022), (8) Computer Aided Simulation of Dynamic Processes (Autumn Semesters 2019-2022), (9) Mathematics III (Differential Equations) (Autumn Semesters 2021-2022), (10) Physics II (Electricity - Magnetism - Electromagnetism) (Spring Semester 2022).

TEACHING STATEMENT
I am able to teach independently several courses, including but not limited to the following list: Chemistry 101, Biochemistry I-II, Bio-Mathematics, Physical Chemistry – Thermodynamics, Spectroscopy, Bio-statistics, Computational Biology, Structural Biology, Programming, Protein Structure and Function, Simulation of Biological Systems: Structure and Function prediction

europass

Βαγγέλης Δασκαλάκης

Ημερομηνία γέννησης: 24/12/1978 | **Υπηκοότητα:** Ελληνική | **Φύλο:** Άντρας |

Αριθμός τηλεφώνου: (+30) 6942436906 (Κινητό τηλέφωνο) | **Αριθμός τηλεφώνου:** (+30) 2610997820 (Εργασία) | **Ηλεκτρονική διεύθυνση:** vdaskalakis@upatras.gr |

Ηλεκτρονική διεύθυνση: vdaskalakis@iceht.forth.gr | **ORCID:** https://orcid.org/0000-0001-8870-0850 |

Διεύθυνση: Πανεπιστήμιο Πατρών, Καραθεοδωρή 1, Πανεπιστημιούπολη, GR 265 04, Πατρα, Ελλάδα (Εργασία)

ΛΊΓΑ ΛΌΓΙΑ ΓΙΑ ΜΈΝΑ

Τόπος γέννησης / Ηράκλειο, Κρήτη-Ελλάδα

ΕΠΑΓΓΕΛΜΑΤΙΚΗ ΕΜΠΕΙΡΙΑ

ΤΜΗΜΑ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ, ΠΑΝΕΠΙΣΤΗΜΙΟ ΠΑΤΡΩΝ – ΠΆΤΡΑ, ΕΛΛΆΔΑ

ΕΠΙΚΟΥΡΟΣ ΚΑΘΗΓΗΤΗΣ – 01/09/2023 – ΤΡΕΧΟΥΣΑ

Βιομοριακή Μηχανική (ΦΕΚ 693/13-3-2023 τ.Γ')

Επιχορηγήσεις Έρευνας:
1. (2025-2026) Proposal No. EHPC-EXT-2025E01-070 **EuroHPC Extreme Scale Access Call** "Digital zoom into the All-atom dynamics of Light-harvesting complexes (DALiA)", 255160 node hours or **20.412.800 core hours MareNostrum5 ACC** (**Accelarated Partition**). Συντονιστής/ Επιστημονικά Υπεύθυνος: Vangelis Daskalakis
2. (2025-2026) Proposal No. EHPC-REG-2025R01-105 **EuroHPC Regular Access Call** "Decoding the Disorder and Promiscuity of Sec14-like SFH Proteins Through Molecular Dynamics (SECure)", 230000 node hours or **25.760.000 CPU-core hrs MareNostrum5 GPP (General Purpose Partition)**. Συντονιστής/ Επιστημονικά Υπεύθυνος: Vangelis Daskalakis
3. (2025) **NAISS** Medium Compute 2025 project (Sweeden) NAISS 2025/5-204 "Sampling the configuration assembly of SFH8 through molecular dynamics", **485300 CPU-core hrs** at Tetralith @ NSC, Συντονιστής: Panagiotis Nikolaou Moschou.
4. (2024-2028) Horizon Europe (HORIZON) Marie Skłodowska-Curie Actions Doctoral Networks (MSCA-DN) 2022, **101119442-PhotoCaM** - "*Photosynthetic Antennas in a Computational Microscope: Training a new generation of computational scientist*" (συνολικός προϋπολογισμός: ***€2.589.847,19***, *Βοηθός Συντονιστής* UPAT ***€240.098,39***; PI: Vangelis Daskalakis).
5. (2024-2025) Ελληνικό Ίδρυμα Έρευνας και Καινοτομίας - ΕΛ.ΙΔ.Ε.Κ. ερευνητική πρόταση No. 14775 SA3. Βιοεπιστήμες - Επιστήμες Ζωής, "SUNDIAL - Seeing Diatoms under a Computational Sunlight". *Συντονιστής* UPAT ***€207.000***; PI: Vangelis Daskalakis
6. (2023-2024) Cyclone 2022A πρόσβαση παραγωγής: **pro22a103s1** - "*Fucoxanthin - chlorophyll protein (FCP): from monomers to tetramers*", **150.000 GLU-core hrs** στο Cyclone. PI: Vangelis Daskalakis
7. (2023-2024) Πρόσβαση παραγωγής No. EHPC-REG-2023R01-128 **EuroHPC Regular Access Call** "*Peptaibols*: *How to kill a bacterium*", **6.400.000 CPU-core hrs** on MeluXina. PI: Vangelis Daskalakis
8. (2024-2026) Χορήγηση Υπερυπολογιστικού χρόνου στο εθνικό σύστημα ARIS HPC (16-18η πρόσκληση):
(a) FCPC - Water/ Proton Conductance in the FCP Light Harvesting Complexes of Diatoms (PI, 1.000.000 GPU core-hrs)
(b) GemT – Molecular dynamics of bacterial gemcitabine transporters (συνεργάτης, 2.000.000 CPU core-hrs)
(c) MultiEng: Engineering multifunctional biocatalysts for the valorization of lignocellulosic biomass (συνεργάτης, 1.500.000 CPU core-hrs)
(d) PscAC: PscA-PscC dynamics in the green sulfur bacteria photosynthetic machinery (συνεργάτης, 700.000 GPU core-hrs)
(e) FanPath: Allosteric Communication and R-Loop Dynamics in Eukaryotic RNA-Guided Nucleases (PI, 1.500.000 core hrs GPU node island)

ΠΑΝΕΠΙΣΤΗΜΙΟ ΠΑΤΡΩΝ – Ρ'ΙΟ, ΠΆΤΡΑ, ΕΛΛΆΔΑ

ΕΠΙΣΚΕΠΤΗΣ ΜΕΛΟΣ ΔΕΠ ΣΤΟ ΙΤΕ/ΙΕΧΜΗ – 07/03/2025

Ίδρυμα Τεχνολογίας Έρευνας / Ινστιτούτο Επιστημών Χημικής Μηχανικής (*ITE/ IEXMH*)

ΤΜΗΜΑ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ, ΤΕΧΝΟΛΟΓΙΚΟ ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΥΠΡΟΥ – ΛΕΜΕΣΌΣ, ΚΎΠΡΟΣ

ΑΝΑΠΛΗΡΩΤΗΣ ΚΑΘΗΓΗΤΗΣ – 01/05/2022 – 31/08/2023

Επιχορηγήσεις Έρευνας:
1. European High-Performance Computing Joint Undertaking (**EuroHPC JU**) πρόγραμμα **EHPC-REG-2021R0021** "*Peptaibols: How to kill a bacterium*", στον Υπερυπολογιστή MeluXina (Λουξεμβούργο), 2.0 mn std-cpu-core hrs, ως συντονιστής (**Απρ 2022 – Οκτ 2022**)
2. Erasmus+ Ατομική Κινητικότητα Εκμάθησης – Κινητικότητα μελών ΔΕΠ για διδασκαλία και εκμάθηση, Queen Mary University of London (**Μάης 2022**)

ΤΜΗΜΑ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ , ΤΕΧΝΟΛΟΓΙΚΟ ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΥΠΡΟΥ – ΛΕΜΕΣΌΣ, ΚΎΠΡΟΣ

ΕΠΙΚΟΥΡΟΣ ΚΑΘΗΓΗΤΗΣ – 31/12/2014 – 30/04/2022

Επιχορηγήσεις Έρευνας:
1. 13th Call **Cyclone** (**Ινστιτούτο Κύπρου**) - "Molecular Dynamics of LHCII trimer complex at quenched and light harvesting states based on Free Energy Minima" (~1.0mn std-cpu core hrs), συντονιστής (**Απρ 2021 – Μαρ 2022**).
2. **GRnet 10th** Project ARIS CYP2D6-DYN "Correlation between CYP2D6 variants and their metabolic activity by Molecular Dynamics Simulations" (3.5mn std-cpu core hrs), συνεργάτης (**Μαρ 2021 – Φεβ 2022**)
3. **PRACE DECI-16 16DECI0015 DynLHCX** "The structure and dynamics of the photoprotective protein LHCX1 in diatoms" 5.0mn std-cpu core hrs, *συντονιστής* (**Ιουν 2020 – Μάη 2021**).
4. **PRACE COVID-19 COVID19-41** "Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution", επιχορήγηση σε υπολογιστικό χρόνο 18.0mn std-cpu core hrs @Joliot-Curie Rome (CEA/GENCI, France) (**Μάη 2020 – Νοε 2021**)
5. COST Action CA18234: "Computational materials sciences for efficient water splitting with nanocrystals from abundant elements", Επιτροπή Διαχείρισης (**Απρ 2020 – 2024**), μέλος Δέσμης Ενεργειών 2 – *Προσομοιώσεις Μοριακής Δυναμικής*.
6. **PRACE DECI-15 15DECI0328 LHCPSSalt** "LHCII-PsbS complex conformations under varying salt content" ~4.0mn std-cpu core hrs, *συντονιστής* (**June 2019 – May 2020**).
7. **PRACE project 2018194641** επιχορήγηση σε υπολογιστικό χρόνο 17.0mn std-cpu core hrs @SuperMUC HPC (Leibniz Supercomputing Centre). "CDynLHCII - Clustering Dynamics of the major Light Harvesting Complexes (LHCII) of Photosystem II under Photoprotection", *συντονιστής* (**Απρ 2019 – Μαρ 2020**).
8. Ίδρυμα Προώθησης Έρευνας (Κύπρος) **POST-DOC/0916/0049 (~160.000 Ευρώ) «***Ενεργοποίηση της Φωτοπροστασίας στις πρωτεΐνες-κεραίες του Φωτοσυστήματος II με Μοριακές Προσομοιώσεις και Φασματοσκοπία Raman*» συντονιστής (**Οκτ 2018 – Μαρ 2022**).
9. Interreg Ελλάδας-Κύπρου, BIOMA «*Αποκεντρωμένη διαχείριση των βιοαποβλήτων και αξιοποίησή τους με χρήση εναλλακτικών και καινοτόμων συστημάτων επεξεργασίας*».
10. Διεθνικό πρόγραμμα κινητικότητας HPC-Europa3 (HPC17K4FRZ, 672.000 std cpu-core hrs) και Ομάδα Ερευνητικής Εργασίας Προσομοίωσης Συστημάτων με Κβαντική Μηχανική (TRG-qm3, 2019) κατά τη Σαββατική άδεια (2018, 2019). Τμήμα Φυσικής και Επιστημών Γης (Τομέας Βιοφυσικής), Πανεπιστήμιο Jacobs, Βρέμη, Γερμανία (**Σεπτ 2018 – Φεβ 2019**).
11. Cy-Tera-LinkSCEEM, PRACE HPC, GRnet ARIS επιχορηγήσεις σε υπολογιστικό χρόνο (*standard core-hours*) ~7.0mn συνολικά για τα ερευνητικά προγράμματα: pro14b114s1, pro14b105s1 and pro15a113s1, pro15b104, pro16a105, pro16b103, pro17a103, pro17b101, , lspre400, lspre410, , **PRACE DECI-13** LHCFlex, **PRACE DECI-14** AIMDPSII, GRnet preparatory ARIS "ADHDyn" & "LHCIIPsbS" *ως συντονιστής*. **GRnet 7th Call** ARIS project "LHCIICRYSTAL" 3.0 mn std cpu-core hrs, *συνεργάτης*.
12. COST Action CM1401: Our Astro-Chemistry History. Επιτροπή Διαχείρισης (Απρ 2015 - Μαρ 2020).
13. Επιχορήγηση κινητικότητας Erasmus για εκπαίδευση (επισκέπτης στην Ακαδημία Επιστημών της Τσεχίας, Ινστιτούτο Οργανικής Χημείας και Βιοχημείας, Πράγα). Μάης 2015.

ΤΜΗΜΑ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ , ΤΕΧΝΟΛΟΓΙΚΟ ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΥΠΡΟΥ – ΛΕΜΕΣΌΣ, ΚΎΠΡΟΣ

ΛΕΚΤΟΡΑΣ – 30/11/2010 – 30/12/2014

Επιχορηγήσεις Έρευνας:
1. Εναρκτήρια Χρηματοδότηση, Τεχνολογικό Πανεπιστήμιο Κύπρου (40.000 €)
2. "Activation and reduction of Nitric Oxide (NO) to laughing gas (N_2O) by Nitric Oxide Reductase (NOR) and heme-copper cbb_3 oxidase (Πηγή: Ίδρυμα Προώθησης Έρευνας €133.181. ΤΕΧΝΟΛΟΓΙΑ/ΘΕΠΙΣ/0609/05 (ΒΕ): (2011-2013), ως συνεργάτης (**Μαρ 2011 – Φεβ 2013**)
3. Cy-Tera & LinkSCEEM HPC επιχορηγήσεις υπολογιστικού χρόνου (860.000 ώρες, *standard core-hours*), για τα ερευνητικά προγράμματα: LinkSCEEM lsprob104s1, lspro13a121s1, pro13b113s1, και pro14a120) ως συντονιστής.
4. The Deutscher Akademischer Austauschdienst (DAAD)/ German Academic Exchange Service. Επιχορήγηση για Δικτύωση ASEMUNDUS (συνεργασία Πανεπιστημίων Ασίας/ Ευρώπης).

5. COST Action ES1206: Advanced Global Navigation Satellite Systems tropospheric products for monitoring severe weather events and climate (GNSS4SWEC) – Επιτροπή Διαχείρισης & Μέλος WG2 (λήξη Απρίλιος 2015)

ΙΝΣΤΙΤΟΥΤΟ ΗΛΕΚΤΡΟΝΙΚΗΣ ΔΟΜΗΣ ΚΑΙ ΛΕΙΖΕΡ, ΣΤΟ ΙΔΡΥΜΑ ΤΕΧΝΟΛΟΓΙΑΣ ΚΑΙ ΕΡΕΥΝΑΣ (ITE) – ΕΛΛΑΔΑ – ΗΡΆΚΛΕΙΟ, ΚΡΉΤΗ, ΕΛΛΆΔΑ

ΕΡΕΥΝΗΤΙΚΟΣ ΣΥΝΕΡΓΑΤΗΣ – 2006 – 2010

Υποτροφία (GRID COMPUTATIONAL CHEMISTRY – GRID-COMPCHEM – Marie-Curie Host Fellowship for the Transfer of Knowledge **EU ToK grant No. MTKD-CT-2005-029583**)

ΥΠΕΡΥΠΟΛΟΓΙΣΤΙΚΟ ΚΕΝΤΡΟ ΤΗΣ ΒΑΡΚΕΛΩΝΗΣ (BSC), ΤΜΗΜΑ ΦΥΣΙΚΩΝ ΕΠΙΣΤΗΜΩΝ ΚΑΙ ΕΠΙΣΤΗΜΩΝ ΖΩΗΣ – ΒΑΡΚΕΛΏΝΗ, ΙΣΠΑΝΊΑ

ΜΕΤΑΔΙΔΑΚΤΟΡΙΚΟΣ ΕΠΙΣΚΕΠΤΗΣ

GRID COMPUTATIONAL CHEMISTRY – GRID-COMPCHEM – Marie-Curie Host Fellowship for the Transfer of Knowledge **EU ToK grant No. MTKD-CT-2005-029583 & Υποτροφία HPC-Europa2**

ΕΚΠΑΙΔΕΥΣΗ ΚΑΙ ΚΑΤΑΡΤΙΣΗ

30/09/1996 – 20/07/2000 Ηράκλειο, Ελλάδα
ΠΤΥΧΙΟ ΧΗΜΕΙΑΣ ΤΜΗΜΑ ΧΗΜΕΙΑΣ, ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

Υποτροφίες:
(1) Εισαγωγής στο Τμήμα Χημείας Βραβείο - Υποτροφία ΙΚΥ (1996), (2) $1^{ο}$,$2^{ο}$,$3^{ο}$ & $4^{ο}$ έτος Υποτροφία Αριστείας ΙΚΥ (1996-2000), (3) $3^{ο}$ Έτος Βραβείο Αριστείας (Δήμος Ηρακλείου), (4) Βραβείο Αριστείας (Πτυχίο), Πανεπιστήμιο Κρήτης - Τμήμα Χημείας (2000).

Διεύθυνση Βούτες, 715 00, Ηράκλειο, Ελλάδα | **Τομέας σπουδών** Χημεία | **Τελικός βαθμός** 8.87/10

06/2000 – 07/2006 Heraklion, Ελλάδα
ΔΙΠΛΩΜΑΤΑ MASTER'S - PH.D ΤΜΗΜΑ ΧΗΜΕΙΑΣ, ΠΑΝΕΠΙΣΤΗΜΙΟ ΚΡΗΤΗΣ

Τίτλος Msc: «Ο μηχανισμός της σχάσης του δεσμού O-O στην κυτοχρωμική *c* Οξειδάση με τη εφαρμογή της Θεωρίας του συναρτησιακού της ηλεκτονιακής πυκνότητας και φασματοσκοπίας συντονισμού *Raman*».
Τίτλος Ph.D: «Βιοενεργετικοί μηχανισμοί του O_2 και του NO με την εφαρμογή της θεωρίας του συναρτησιακού της ηλεκτρονιακής πυκνότητας».

(1) Grant-in-Aid for Scientific research (Grant-in-Aid for Specially Promoted Research) FY2005. ***Επισκέπτης υποψήφιος διδάκτορας* - Ινστιτούτο Βιοεπιστημών Εθνικού Ινστιτούτου Φυσικών Επιστημών, Υπερυπολογιστικό Κέντρο**, **Οκαζάκι, Αΐτσι / Ιαπωνία** (2005).
(2) Υποτροφία ΙΚΥ για την εισαγωγή στο μεταπτυχιακό πρόγραμμα (2001-2002), (2) Υποτροφία **Μαρίας Μανασάκη** (2001-2002, 2002-2003).
(3) *Τίτλος Προγράμματος:* ***Δυναμική και δραστικότητα των ενζυμικών διεργασιών που περιλαμβάνουν την*** aa_3 ***αιμο-χαλκο οξειδάση από το P. denitrificans: Φασματοσκοπία και Θεωρητικοί Υπολογισμοί***
Χρηματοδότηση: ***Υπουργείο Παιδείας (Ελλάδα) - Πυθαγόρας Ι (2006)***
(4) *Τίτλος Προγράμματος:* ***Βιοενεργετικοί Μηχανισμοί του*** O_2 ***και του NO με την εφαρμογή της θεωρίας του συναρτησιακού της ηλεκτρονιακής πυκνότητας***
Χρηματοδότηση: ***Υπουργείο Παιδείας / Ε.Ε. Ηράκλειτος (2002-2005)***
(5) *Τίτλος Προγράμματος:* ***Δομική μελέτη της αναγωγάσης του μονοξειδίου του αζωτου (nor)***
Χρηματοδότηση: ***Υπουργείο Παιδείας (Ελλάδα), Γενική Γραμματεία Έρευνας και Τεχνολογίας ΓΓΕΤ (2000-2001)***

Διεύθυνση Βούτες, Ηράκλειο, 715 00, Heraklion, Ελλάδα | **Τομέας σπουδών** Υπολογιστική Βιοφυσική Χημεία |

Τελικός βαθμός 9.75/10

ΓΛΩΣΣΙΚΕΣ ΔΕΞΙΟΤΗΤΕΣ

Μητρική γλώσσα/-ες: **ΕΛΛΗΝΙΚΑ**

Άλλη/-ες γλώσσα/-ες:

	ΚΑΤΑΝΟΗΣΗ		ΟΜΙΛΙΑ		ΓΡΑΦΗ
	Ακρόαση	Ανάγνωση	Παραγωγή λόγου	Επικοινωνία λόγου	
ΑΓΓΛΙΚΑ	C2			C2	C2

	ΚΑΤΑΝΟΗΣΗ		ΟΜΙΛΙΑ		ΓΡΑΦΗ
	Ακρόαση	Ανάγνωση	Παραγωγή λόγου	Επικοινωνία λόγου	
ΓΑΛΛΙΚΑ	B1			B1	B1

Επίπεδα: A1 και A2: Βασικός χρήστης· B1 και B2: Ανεξάρτητος χρήστης· C1 και C2: Έμπειρος χρήστης

ΕΡΕΥΝΑ

ΤΡΕΧΟΥΣΑ

Αποδοτικότητα

53 δημοσιεύσεις ως άρθρα σε περιοδικά με ομότιμη κρίση (46), κεφάλαια βιβλίων (6) και πρακτικά συνεδρίων. **Πρώτος συγγραφέας σε 23/53** και **αλληλογραφών συγγραφέας σε 23/53** δημοσιεύσεις, παρουσιάζοντας ισχυρή ερευνητική ανεξαρτηρία (h-index Scopus 17, Google Scholar 22, i10-index 31). Δημοσιεύσεις σε κορυφαία περιοδικά στους τομείς της βιοφυσικής χημείας, φυσικοχημείας και βιομοριακής Δυναμικής (π.χ. J. Am. Chem. Soc. Proc. Natl. Acad. Sci USA, Biochim. Biophys. Acta, NPG Commun. Chem., Sci. Rep., J. Phys. Chem. B-C, Phys. Chem. Chem. Phys., Chem. Commun., J. Biomolecular Struct. and Dynamics). Ομότιμος κριτής σε περιοδικά, όπως Nature Journals, ACS Physical Chemistry Journals, RSC Phys. Chem. Chem. Phys., RSC Advances, Springer J. Molecular Modeling (περισσότερες από 270 κρίσεις σε περιοδικά, Web of Science – publons, **Outstanding Reviewer for Phys. Chem. Chem. Physics 2024**; Phys. Chem. Chem. Phys. 2025, 27, 12111-12111). Ομότιμος κριτής για ερευνητικές προτάσεις σε κέντρα Υπερυπολογιστών (High Performance Computing, HPC) όπως CyTera και Cyclone στο Ινστιτούτο Κύπρου, GRNET ARIS HPC - the National Infrastructures for Research and Technology, CSCS-Swiss National Supercomputing Centre, Institute for Advanced Simulation (IAS), Jülich Supercomputing Centre (JSC), Gauss Centre for Supercomputing (GCS) and the John von Neumann Institute for Computing (NIC)). Κριτής για το Biotechnology and Biological Sciences Research Council (BBSRC) και το Czech Science Foundation. **44 συμμετοχές σε Διεθνή Συνέδρια** - Σεμινάρια, περιλαμβανομένων **13 διαλέξεων με πρόσκληση** . Η ερευνητική μου δραστηριότητα έχει περιληφθεί στο περιοδικό PRACE DIGEST (Insight Publishers) τα έτη 2017, 2020.

Εργαστήριο Βιομοριακής Δυναμικης και Μηχανικής

Η ανεξάρτητη ερευνητική μου δραστηριότητα επικεντρώνεται σε μελέτες βιοφυσικής χημείας μεγάλων βιολογικών μορίων που συμμετέχουν σε διαδικασίες σχετιζόμενες με τις επιστήμες ζωής (Βιολογία, Βιομοριακή Μηχανική):
Heme proteins, Photosystem II Light Harvesting Complexes, SARS-CoV-2 proteins, Intrinsically Disordered Proteins and Condensates, Protein Thermostability, the CRISPR-Cas and Fanzor systems
Στο εργαστήριο εφαρμόζουμε υπολογιστικές τεχνικές που βασίζονται στη μεθοδολογία της Μοριακής Δυναμικής (MD) , όπως η επιταχυνόμενη δυναμική (accelarated MD), η μεταδυναμική πολλαπλών βημάτων, ή η μεταδυναμική παράλληλης ανταλλαγής στο ομαλά-συγκλίνον στατιστικό σύνολο, σε συνδυασμό με την κβαντική μέθοδο του Συναρτησιακού της Ηλεκτρονιακής Πυκνότητας (DFT). Το στήσιμο των μοντέλων και η ανάλυση των αποτελεσμάτων (τροχιών MD) βασίζεται σε εργαλεία βιοπληροφορικής (αλγόριθμοι αλληλεπίδρασης πρωτεΐνης με πρωτεΐνη, δομική ευθυγράμμιση και αλληλουχική ομολογία, μοντέλα Markov State). Για την έρευνά μας, χρησιμοποιούμε υπερυπολογιστικά συστήματα (HPC, Joliot Curie - Irene ROME TGCC στη Bruyères-le-Châtel, Salomon iT4i στην Τσεχία, SuperMUC-NG LRZ στο Μόναχο, HLRS στη Στουτγάρδη, MareNostrum στο Υπερυπολογιστικό Κέντρο της Βαρκελώνης) στο πλαίσιο των επιχορηγούμενων προγραμμάτων EuroHPC JU (https://www.eurohpc-ju.europa.eu), PRACE/ DECI (https://prace-ri.eu/). Η διττή οπτική που παρέχει ο συνδυασμός υπολογιστικών και πειραματικών τεχνικών βιοχημείας, βιοφυσικής και βιολογικής χημείας καθιστά την ομάδα μου μια από τις πιο κατάλληλες να μελετήσουν απαιτητικούς ερευνητικούς στόχους.

ΔΗΜΟΣΙΕΥΣΕΙΣ

01. Conformational plasticity enables functional switching in diatom lightharvesting complexes

Sousani TI, Zender B, Maity S, Kleinekathöfer U, and **Daskalakis V*** (2025) ***Commun Chem*** 8, 392 https://doi.org/10.1038/s42004-025-01774-x

02. An Unexpected Water Channel in the Light-Harvesting Complex of a Diatom: Implications for the Switch between Light Harvesting and Photoprotection

Daskalakis V*, Maity S and Kleinekathöfer U (**2025**) ***ACS Phys. Chem Au*** 5, 1, 47–61. *doi:* 10.1021/acsphyschemau.4c00069 (***January 2025 Journal Cover***)

03. Hydrophobic mismatch in the thylakoid membrane regulates photosynthetic light harvesting

Wilson S, Clarke C, Carbajal MA, Buccafusca R, Fleck R, **Daskalakis V**, and Ruban, A***** (**2024**) ***J. Am. Chem. Soc.*** 146, 21, 14905–14914**.** DOI: 10.1021/jacs.4c05220

04. Acclimation mechanism of microalgal photosynthetic apparatus under low atmospheric pressures – New astrobiological perspectives in a Mars like atmosphere

Gritsi CS, Sarmas E, **Daskalakis V** and Kotzabasis K* (2024) ***Functional Plant Biology*** 51, FP24058, doi:10.1071/FP24058

05. Electric Field Susceptibility of Chlorophyll c Leads to Unexpected Excitation Dynamics in the Major Light-Harvesting Complex of Diatoms

Maity S, **Daskalakis V**, Jansen LCT, and Kleinekathöfer U* (**2024**) ***J. Phys. Chem. Lett.*** 15, 9, 2499–2510

06. The synergy between the PscC subunits for electron transfer to the P840 special pair in Chlorobaculum tepidum

Daskalakis V, Lyratzakis A, Xie H, and Tsiotis G* (**2024**) ***Photosynth Res*** 160, 87–96. doi: 10.1007/s11120-024-01093-7

07. Engineering salt-tolerant Cas12f1 variants for gene-editing applications

Daskalakis, V* and Papapetros, S (**2023**) **J. Biomolecular Struct. and Dynamics**, , doi: 10.1080/07391102.2023.2240418

08. Recognition motifs for Importin 4 [(L)PPRS(G/P)P] and Importin 5 [KP(K/Y)LV] bind-ing, identified by bio-informatic simulation and experimental in vitro validation

Panagiotopoulos AA, Kalyvianaki K, Tsodoulou PK, Darivianaki MN, Dellis D, Notas G, **Daskalakis V**, Theodoropoulos PA, Panagiotidis CA, Castanas E, Kampa M* (**2022**) **Comp. Struct. Biotechnol. J.** doi: 10.1016/j.csbj.2022.10.015

09. Deciphering the QR code of the CRISPR-Cas9 system: Synergy between Gln768 (Q) and Arg976 (R)

Daskalakis V* (**2022**) ***Journal of Physical Chemistry Au***. doi: 10.1021/acsphyschemau.2c00041

10. Trivial Excitation Energy Transfer to Carotenoids is an Unlikely Mechanism for Non-Photochemical Quenching in LHCII

Gray C, Wei T, Polívka T, **Daskalakis V**, and Duffy CDP* (**2022**) ***Front. Plant Sci.*** 12: 797373.

11. Robust Strategy for Photoprotection in the Light-Harvesting Antenna of Diatoms: A Molecular Dynamics Study

Chrysafoudi A, Maity S, Kleinekathöfer U and **Daskalakis V*** (**2021**) **J. Phys. Chem. Lett.** 12, 9626−9633

12. Natural polyphenols inhibit the dimerization of the SARS-CoV-2 main protease: the case of fortunellin and its structural analogs

Panagiotopoulos AA, Karakasiliotis I, Kotzampasi D-M, Dimitriou M, Sourvinos G, Kampa M, Pirintsos S, Castanas E* and **Daskalakis V*** (**2021**), **Molecules** (**MDPI**), *26, 6068.*

13. Time-Dependent Atomistic Simulations of the CP29 Light-Harvesting Complex

Maity S, Sarngadharan P, **Daskalakis V**, and Kleinekathöfer U* (**2021**), ***J. Chem. Phys.*** 155, 055103

14. Hydrogen gas as a central on-off functional switch of reversible metabolic arrest – New perspectives for biotechnological applications

Zerveas S, Kydonakis E, Mente M-S, **Daskalakis V**, and Kotzabasis K (**2021**) **J. Biotechnology**, *335, 9 - 18*

15. p-cymene impairs SARS-CoV- 2 and Influenza A (H1N1) viral replication: In silico predicted interaction with SARS-CoV- 2 nucleocapsid protein and H1N1 nucleoprotein

Panagiotopoulos A, Tseliou M, Karakasiliotis I, Kotzampasi D-M, **Daskalakis V**, Kesesidis N, Notas G, Lionis C, Kampa M, Pirintsos S, Sourvinos G, Castanas E. (**2021**) ***Pharmacol Res Perspect.*** 9:e00798

16. Multiscale QM/MM Molecular Dynamics Simulations of the Trimeric Major Light-Harvesting Complex II

Maity S, **Daskalakis V**, Elstner M and Kleinekathöfer U* (**2021**) ***Phys. Chem. Chem. Phys***, 23, 7407 – 7417

17. The conformational phase space of the photoprotective switch in the major Light Harvesting Complex II

Daskalakis V*, Papadatos S, Stergiannakos, **(2020) Chem. Commun.** 56, 11215 – 11218

18. Structure and Dynamics of a Thermostable Alcohol Dehydrogenase from the Antarctic Psychrophile Moraxella sp. TAE123

Petratos K*, Gessmann R, **Daskalakis V**, Papadovasilaki M, Papanikolau Y, Tsigos I , and Bouriotis V **(2020) ACS Omega**, 5, 24, 14523–14534

19. Structural Basis for Allosteric Regulation in the Major Antenna Trimer of Photosystem II

Daskalakis V*, Maity S, Hart CL, Stergiannakos T, Duffy CDP, and Kleinekathöfer U **(2019)** ***J. Phys. Chem. B,*** *123*, 45, 9609-9615

20. Fine tuning of the photosystem II major antenna mobility within the thylakoid membrane of higher plants

Daskalakis V*, Papadatos S, Kleinekathoefer, U (**2019**) ***Biochim. Biophys. Acta – Biomembranes*****,** *1861*, 183059

21. On a Chlorophyll-Carotenoid Coupling in LHCII

Maity S, Gelessus A, **Daskalakis V**, Kleinekathoefer, U* (**2019**) ***Chem. Phys.*** *526,* 110439

22. Protein-Protein Interactions within Photosystem II under Photoprotection: The Synergy between CP29 Minor Antenna, Subunit S (PsbS) and Zeaxanthin at all-atom resolution

Daskalakis V* (**2018**) ***Phys. Chem. Chem. Phys.*** *20*, 11843 – 11855

23. The Photosystem II Subunit S under Stress

Daskalakis V*, and Papadatos S (**2017**) ***Biophys. J. (Cell)*** *113 (11)*, 2364-2372.

24. A pathway for protective quenching in antenna proteins of Photosystem II

Papadatos S, Charalambous C A, and **Daskalakis V*** (**2017**) ***Scientific Reports (NPG)*** *7,* 2523. doi: 10.1038/s41598-017-02892-w.

25. Detection of Maillard reaction products by a coupled HPLC-Fraction collector technique and FTIR characterization of Cu(II)-complexation with the isolated species

Ioannou A, **Daskalakis V**, and Varotsis C* (**2017**) ***J. Mol. Struct.*** *1141*, 634–642.

26. Coupling of helix E-F motion with the O-nitrito and 2-nitrovinyl coordination in myoglobin

Ioannou A, Lambrou A, **Daskalakis V*** and Pinakoulaki E* (**2017**) ***Biophys. Chem.*** *221,* 10-16.

27. Nitrite coordination in myoglobin

Ioannou A, Lambrou A, **Daskalakis V** and Pinakoulaki E* (**2017***) **J. Inorg. Biochemistry (JIB)**, 166, 49-54.*

28. Energizing the Light Harvesting Antenna: Insight from CP29

Ioannidis NE, Papadatos S, and **Daskalakis V*** (**2016**) ***BBA – Bioenergetics***, *1857 (10), 1643-1650.*

29. Correlation Between Surface Tension and the Bulk Dynamics in Salty Atmospheric Aquatic Droplets

Salameh A, Vorka, F, and **Daskalakis V* (2016)** ***J. Phys. Chem. C***, *120 (21), 11508-11518*

30. Structure and properties of the catalytic site of nitric oxide reductase at ambient temperature

Daskalakis V, Ohta T, Kitagawa T, Varotsis C* **(2015)** ***Biochim. Biophys. Acta – Bioenergetics***, 1847(10), 1240–1244.

31. Surface-Active Organic Matter induces salt morphology transitions during new atmospheric particle formation and growth

Daskalakis V*, Charalambous F, Demetriou DC, Georgiou AG **(2015)** ***RSC Adv.***, 5, 63240–63251.

32. Effects of Surface Activity on Carbon Dioxide Nucleation in Atmospheric Wet Aerosols: A Molecular Dynamics Study

Daskalakis V*, Charalambous F, Panagiotou F, Nearchou I **(2014)** ***Phys. Chem. Chem. Phys.***, 16: 23723-23734.

33. Hexagonal Ice Stability and Growth in the presence of Glyoxal and Secondary Organic Aerosols

Daskalakis V*, Hadjicharalambous M **(2014)** ***Phys. Chem. Chem. Phys.*** 16(33): 17799-17810.

34. The protein effect in the structure of two ferryl-oxo intermediates at the same oxidation level in the heme-copper binuclear center of cytochrome c oxidase

Pinakoulaki E, **Daskalakis V**, Ohta T, Richter O M, Budiman K, Kitagawa T, Ludwig B, Varotsis C* **(2013)** ***J. Biol. Chem.*** 288(28): 20261-20266.

35. Exploring the Topography of Free Energy Surfaces and Kinetics of Cytochrome c Oxidases interacting with small ligands

Porrini M, **Daskalakis V**, Farantos SC* **(2012)** ***RSC Adv.*** 2: 5828 - 5836.

36. Non-Linear Vibrational Modes in Biomolecules: a periodic orbits description

Kampanarakis A, Farantos SC*, **Daskalakis V** and Varotsis C **(2012)** ***Chem. Phys. Elsevier***, 399: 258–263.

37. The origin of the FeIV=O intermediates in cytochrome aa3 oxidase

Pinakoulaki E, **Daskalakis V** and Varotsis C* **(2012)** ***BBA Bioenergetics***, 1817: 552-557.

38. Regulation of Electron and Proton Transfer by the Protein Matrix of Cytochrome c Oxidase

Daskalakis V, Farantos SC, Guallar V, Varotsis C* (**2011**) ***J. Phys. Chem. B***, 115(13): 3648-3655

39. Vibrational Resonances and CuB displacement controlled by proton motion in Cytochrome c Oxidase

Daskalakis V*, Farantos SC, Guallar V, Varotsis C (**2010**) ***J. Phys. Chem. B***, 114(2): 1136-1143

40. Binding and Docking Interactions of NO, CO and O2 in Heme Proteins as Probed by Density Functional Theory

Review for the Special Issue on "Application of Density Functional Theory in Chemical Reactions"
Daskalakis V, Varotsis C* (**2009**) ***Int. J. Mol. Sci.,*** 10: 4137-4156

41. Heme Cavity Dynamics of Photodissociated CO from ba3-Cytochrome c Oxidase: The Role of Ring-D Propionate

Porrini M*, **Daskalakis V**, Farantos SC, Varotsis C *(***2009**) ***J. Phys. Chem. B***, 113(35): 12129-12135

42. Assigning vibrational spectra of ferryl-oxo intermediates of cytochrome c oxidase by periodic orbits and Molecular Dynamics

Daskalakis V, Farantos SC*, Varotsis C *(***2008***) **J. Am. Chem. Soc*** 130(37): 12385-12393

43. Probing the environment of CuB in heme-copper oxidases

Daskalakis V, Pinakoulaki E, Stavrakis S, Varotsis C* (**2007**) ***J. Phys. Chem. B*** 111: 10502-10509

44. Two ligand binding sites in the O2-sensing signal transducer HemAT: Implications for ligand Recognition/ Discrimination and signaling

Pinakoulaki E, Yoshimura H, **Daskalakis V**, Yoshioka S, Aono S, Varotsis C* (**2006**) ***Proc. Natl. Acad. Sci. USA*** 103: 14796-14801

45. Structural dynamics of Heme-copper oxidases and Nitric oxide reductases: Time-Resolved step-scan FTIR and Time-resolved Resonance Raman studies

Pinakoulaki E, Koutsoupakis C, Stavrakis S, Marialena A, Papadopoulos G, **Daskalakis V**, Varotsis C* (**2005**) ***J. Raman Spec.*** 36: 337-349

46. Time-resolved step-scan Fourier transform infrared investigation of heme-copper oxidases: implications for O2 input and H2O/H+ output channels

Koutsoupakis C, Pinakoulaki E, Stavrakis S, **Daskalakis V**, Varotsis C* (**2004**) ***Bioch. Biophys. Acta*** 1655: 347-352

ΑΡΘΡΑ ΑΝΑΣΚΟΠΗΣΗΣ/ ΚΕΦΑΛΑΙΑ ΒΙΒΛΙΩΝ----------

47. From Traditional Ethnopharmacology to Modern Natural Drug Discovery: A Methodology Discussion and Specific Examples

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Pirintsos S, Panagiotopoulos A, Bariotakis M, **Daskalakis V**, Lionis C, Sourvinos G, Karakasiliotis I, Kampa M, and Castanas E. (**2022**) ***MDPI Molecules***, 27(13), 4060.

48. A perspective on the Major Light Harvesting Complex Dynamics Under the Effect of pH, Salts and the Photoprotective PsbS Protein

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Navakoudis E, Stergiannakos T, and **Daskalakis V*** (**2022**) *Quantum and classical computational methods in photosynthesis: from the atom to the mesoscale* in ***Photosynthesis Research**, in press*

49. Atmospheric Ice Nucleation by Glassy Organic Compounds: A Review

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Salameh A, and **Daskalakis V*** (**2017**), **Chem. Comp. J** 1(1): 13-23

50. Probing the Action of Cytochrome c Oxidase (2014) The Structural Basis of Biological Energy Generation

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Daskalakis V, Varotsis C* **Advances in Photosynthesis and Respiration**, 39 (10): SBN 978-94-017-8742-0

51. Tuning heme functionality: the cases of Cytochrome c Oxidase and Myoglobin Oxidation

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Daskalakis V*, Farantos S C, Varotsis C **(2012), LNCS – Springer-Verlag Berlin, Heidelberg**, p. 304-315. ISBN: 978-3-642-31124-6

52. Grid Computing Multiple Shooting Algorithms for Extended Phase Space Sampling and Long Time Propagation in Molecular Dynamics

Κεφάλαιο σε Βιβλίο/ Ανασκόπηση: Daskalakis V, Giatromanolakis M, Porrini M, Farantos, SC* and Gervasi O ***Computer Physics**, Chapter 4 pp. 1-18, **2011** © Nova Science Publishers,* Inc. *Editors: B. S. Doherty, A. N. Molloy.* ISBN 978-1-61324-790-7

53. Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach

Πρακτικά Συνεδρίου: Daskalakis V*, Farantos SC, Varotsis C (**2007**) ***AIP Computation in Modern Science and Engineering, Proc.*** 963(2): 31-34

ΣΥΝΕΔΡΙΑ ΚΑΙ ΣΕΜΙΝΑΡΙΑ

2023 – 2025

Συνέδρια - Σεμινάρια - Ομάδες Εργασίας

1. Sousani TI, Zender B, Maity S, Kleinekathöfer U and **Daskalakis V*** ″Intrinsic Conformational Plasticity Fine-Tunes Light Harvesting in Diatoms". Extended Hanseatic meeting on Exciton Dynamics and Spectroscopy 2025, Vilnius, Lithouania, September 29 - October 4, 2025 (invited talk).

2. Karvounis IG, Tsiavou V, and **Daskalakis V*** ″Molecular Dynamics of RNA-Guided Endonucleases: Comparative Insights into Cas12 and Eukaryotic Fanzor Systems". The 5th International Symposium on Frontiers in Molecular Science, Kyoto, Japan, August 26-29, 2025.

3. Daskalakis V* ″Baila Morena: The Choreography of Proteins Under a Computational Microscope". ICFO FRONTIERS RESEARCH SCHOOL: Physics for Biology and Medicine, Barcelona, Spain, July 7-11 2025 (invited talk).

4. Theofani-Iosifina Sousani and **Daskalakis V*** ″Light-induced transfer of a proton in the light-harvesting complexes of diatoms". ACS Spring 2025 Meeting & Expo, San Diego, CA, USA, March 23-27.

5. Daskalakis V*, Maity S, Kleinekathöfer U. ″Diatoms under Computational Sunlight". Second European Congress on Photosynthesis Research (ePS2 2024), Padova, Italy, 25-28 June 2024.

6. Karampa P, Makryniotis K, Nikolaivits E, **Daskalakis V**, Topakas E, Dimarogona M*. ″Investigation of Structural Determinants of Plastic Degrading Enzymes via x-ray Crystallography and Molecular Docking". 14ο Πανελλήνιο Επιστημονικό Συνέδριο Χημικής Μηχανικής, Θεσσαλονίκη, Ελλάδα, 29-31 Μάη 2024.

7. Daskalakis V. "CRISPR-Cas proteins: Engineering of "silver-bullets" in the arsenal of gene editing". International Society of Quantum Biology and Pharmacology (ISQBP2024) President's Meeting, Athens, Greece, 19-23 May 2024.

8. Daskalakis V. *"Βιομοριακές Προσομοιώσεις: Από τη Δυναμική στη Μηχανική*". Σεμινάριο στο Ίδρυμα Τεχνολογίας και Έρευνας / Ινστιτούτο Επιστημών Χημικής Μηχανικής (ITE/IEXMH), 17 Απρίλη 2024 (προσκλεκλημένη ομιλία)

9. Daskalakis V. *"Biomolecular Engineering: Structures and Dynamics*". Seminar at the Department of Physics, Constructor University, Bremen, Germany, 27 April 2023 (*invited talk*)

10. Daskalakis V. *"Biomolecular Engineering: Structures and Dynamics*". Σεμινάριο στο Ελληνικό Κέντρο Θαλάσσιων Ερευνών (ΕΛ.ΚΕ.Θ.Ε) στο Ινστιτούτο Θαλάσσιας Βιολογίας, Βιοτεχνολογίας και Υδατοκαλλιεργειών (Ι.ΘΑ.Β.Β.ΥΚ), Ηράκλειο, Ελλάδα, 03 Μάη 2023 (π*ροσκεκλημένη ομιλία*)

11. Daskalakis V. *"Biomolecular Engineering: Structures and Dynamics*". Σεμινάριο στο Τμήμα Χημείας του Αριστοτελείου Πανεπιστημίου Θεσσαλονίκης, Ελλάδα, 15 May 2023 (π*ροσκεκλημένη ομιλία*)

2020 – 2022

Συνέδρια - Σεμινάρια - Ομάδες Εργασίας

1. Daskalakis V.*"CRISPR-Cas9: From Biomolecular Engineering to Dynamics*". Joint Seminar Series in Biotechnology, Biosciences, and Biomedical Research of the University of Ioannina (School of Medicine), co-organized by IIPPS - Mol Cell Biol Biotechnol, URCI - Institute of Biosciences, IMBB-FORTH, Biomedical Research Dept. (BRI-FORTH), 16 December 2022 (online, *invited talk*)

2. Daskalakis V. *"From Rigid Crystal Structures to Conformational Sampling: A tale of two Light Harvesting Complexes*". Virtual international conference Computational methods in photosynthesis: From atoms to the mesoscale, from theory to experiment (ComPhot2021), November 8-11, 2021 (online, *invited talk*)

3. Daskalakis V. *"From Rigid Crystal Structures to Conformational Sampling: A tale of two Light Harvesting Complexes*". Virtual HPC-Europa3 TAM Meeting, November 3-4, 2021 (online talk)

4. Daskalakis V. "The mechanics of photoprotection in the major antenna of Photosystem II: let there be light...", SuperMUC-NG Status and Results Workshop, 8-10 June 2021 (online, invited talk).

5. Daskalakis V. "High Performance Computing in Structural Biology", CaSToRC - The Cyprus Institute, 19 January 2021 (online, *invited talk*)

6. Daskalakis V. "Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution", EuroHPC Summit Week, 22-26 March 2021 (online, *invited talk*)

2014 – 2020

Συνέδρια - Σεμινάρια - Ομάδες Εργασίας

7. Daskalakis V.COVID-19 pandemic – What have we learned and what does the future hold? Online Seminar, The Cyprus Institute, December 5 2020 (*invited talk*)

8. Daskalakis V., Stergiannakos T., Papadatos, S. **The Synergy between LHCII and PsbS under Photoprotection**, Biophysics of Photosynthesis 2019, Accademia dei Lincei, Rome Italy, October 2-4, 2019

9. Daskalakis V., Stergiannakos T., Papadatos, S. **The Photosynthetic Apparatus under Stress by Molecular Simulations**, Photosynthesis Gordon Research Conference, Grand Summit Hotel at Sunday River in Newry, ME United States, July 21-16, 2019 *(by invitation only).*

10. Daskalakis V. Lecture, **Fine Tuning of the Photosynthetic Apparatus**, Department of Materials Science and Technology, Heraklion, Greece, 20 May 2019 *(invited talk).*

11. Daskalakis V. Lecture, **The Photosynthetic Apparatus under Stress by Molecular Simulations**, National Hellenic Research Foundation, Athens, Greece, 17 December 2018 *(invited talk).*

12. Daskalakis V. Molife Research Seminar, **Triggering Photoprotection in Photosystem II Light Harvesting Complexes by Molecular Simulations**, Bremen, Germany GmbH, 25 September 2018 *(invited talk).*

13. Daskalakis V. 62 nd Annual Meeting Biophysical Society, **S(T)IMULATING THE INTERPLAY BETWEEN PHOTOSYSTEM II PROTEINS AND THE XANTHOPHYLL CYCLE IN PHOTOPROTECTION**, San Francisco, USA, 17-21 February 2018

14. Daskalakis V. 3d EMN Meeting on Computation and Theory – Molecular Dynamics and Its Applications, **The effect of proton and potential gradients on integral membrane proteins: Insights from Molecular Dynamics simulations**, Dubai UAE, 6-10 November 2017 (Invited Talk)

15. Daskalakis V, Papadatos S**.** 42nd FEBS Congress (from molecules to cells and back) – **The Photosystem II Subunit S Dynamics under Stress**, Jerusalem Israel, 10-14 September 2017 (Poster).

16. Daskalakis V, Salameh A, AGU 2016 Fall Meeting – ***Correlation Between Surface Tension and the Bulk Dynamics in Salty Atmospheric Aquatic Droplets, San Francisco USA, 12-16 December 2016 (Poster).***

17. Daskalakis V, Department of Chemistry University of Crete Seminars, ***Oxygen Evolution and Reduction: Common Principles***, *Heraklion-Crete, Greece, 25 November 2017 (invited talk).*

18. Daskalakis V, Ioannidis NE, Papadatos S**.** 79th Harden Conference – Oxygen Evolution and Reduction – Common Principles**: Tuning of a conformational change in CP29 from spinach: from Light Harvesting to Photoprotection**, Innsbruck Austria, 16-20 April 2016 (Poster+Talk).

19. Daskalakis V and Pinakoulaki E. New Biological Frontiers Illuminated by Molecular Sensors and Actuators meeting being held in Taipei, Taiwan, June 28 – July 1, 2015. Abstract titled "Globin Nitrito Heme Fe-O-N=O/ 2-Nitrovinyl Species: Impications for Myoglobin Helices Dynamics", fixed-participants meeting.

20. Organizational Committee "12th Greece-Cyprus Conference on Chemistry 2015", 8-10 May 2015, Thessaloniki Greece

2009 – 2014

Συνέδρια - Σεμινάρια - Ομάδες Εργασίας

21. Daskalakis V, Hadjicharalambous M, Charalambous F ***Ice 1_h crystal stability and growth in the presence of glyoxal Secondary Organic Aerosol and Carbon Dioxide***. 13th Quadrennial IGACGP Symposium 13th IGAC Science Conference on Atmospheric Chemistry (IGACGP, IGAC 2014), Brazil, Natal, 22-26 September, 2014.

22. Daskalakis V, Hadjicharalambous M ***Probing the Effects of Atmospheric Pollutants on Ice Nucleation***. International Conference on Scientific Computing 2013 (CSC 2013), Paphos, Cyprus, 3 - 6 December 2013. (Invited talk).

23. Daskalakis V, Varotsis C **The structure of the Hyponitrite in Nitric Oxide Reductase (NOR)**. Biophysical Society (BPS) 57th Annual Meeting in Philadelphia, Pennsylvania, February 2-6, 2013.

24. Daskalakis V, ASEMUNDUS Networking seminar in Korea. Erasmus Mundus programme to enhance quality in higher education through scholarships and academic cooperation between Europe and the rest of the world. Seoul, Korea, May 15-16, 2012.

25. Daskalakis V, Farantos S C, Varotsis C ***Tuning heme functionality: the cases of Cytochrome c Oxidase and Myoglobin Oxidation***, **12th International Conference on Computational Science and Applications** (**ICCSA 2012**), **June 18-21, Salvador de Bahia, Brazil, 2012.** *(Best paper Award)*

26. Daskalakis V, Varotsis C ***Probing the effect of the proximal and distal to the heme a_3 environments in the Cytochrome c Oxidase dioxygen reaction***, 15th International Conference on Biological Chemistry (ICBIC15), 7-12 August, Vancouver, Canada, 2011.

27. CD-ADAPCO, STAR-CCM+ Training School, 10-12 May 2011, London, UK.

28. Daskalakis V, Farantos S C, Guallar V, Varotsis C ***QM/MM Calculations on Cytochrome c Oxidase: Probing of electron and proton pump coupling***, TAM 2010 MEETING, Helsinki 15-17 June 2010.

2001 – 2010

Συνέδρια - Σεμινάρια - Ομάδες Εργασίας

29. Expanding the Frontiers of Molecular Dynamics Simulations in Biology, 23-25 November, Institu d' Estudis Catalans, Barcelona – Spain, 2009 (Joint BSC - IRB Barcelona Conference).

30. Aug. 31 – Sept. 5 2009: Summer School on Simulation Approaches to Problems in Molecular and Cellurar Biology, Miramar Palace, San Sebastian, Spain. **Cecam** (Centre Europeen de Calcul Atomique et Moleculaire), *under* **Psi-K** *scholarship*.

31. Daskalakis V, Farantos S C, Guallar V, Varotsis C ***Towards the Understanding of His411-Fe^{IV}=O Spectroscopic Properties in Ferryl Intermediate of Cytochrome c Oxidase + O_2 Reaction: A Theoretical QM/MM, MD Approach***, 14th International

Conference on Biological Inorganic Chemistry (ICBIC14), 25-30 July, Nagoya, Japan, 2009. ***SBIC (The Society of Biological Inorganic Chemistry)*** *Poster Award for outstanding contribution*.

32. Porrini M**, Daskalakis V**, Farantos SC, Varotsis C ***Heme cavity dynamics of photodissociated CO from ba$_3$-cytochrome c oxidase: The role of ring-D propionate***, 10th Congress in Chemistry Greece – Cyprus, 2-4 July Heraklion, Greece, 2009.

33. a. Daskalakis V, Farantos C S, Varotsis C **Assigning Vibrational Spectra of Ferryl-Oxo Intermediates of Cytochrome *c* Oxidase by Periodic Orbits and Molecular Dynamics,**

b. Daskalakis V, Varotis C **Cytochrome *c* Oxidase + O_2 reaction intermediates as probed by Density Functional Theory: The Proximal and Distal to heme a_3 effects,**

c. Daskalakis V, Varotsis C **Theoretical Studies of Metal-NO*x* species, isolated and in aqueous solutions: Raman bands,** 10th Congress in Chemistry Greece – Cyprus, 2-4 July Heraklion, Greece, 2009.

34. 15-18 Sept. 2008: **Cost Training School On Molecular And Material Science Grid Applications** - Trieste, Italy.

35. Gervasi O, Farantos S C, **Daskalakis V**, Giatromanolakis M ***The Study of cytochrome c Oxidase on the EGEE Grid***, *3d EGEE User Forum*, *Clemont-Ferrand, France, 2008.*

36. Daskalakis V, Giatromanolakis M, Farantos SC, Gerbasi O ***EGEE: Applications in Classical and Quantum Molecular Dynamics,*** *First Hellas Grid User Forum*, *Athens, Greece*, 2007.

37. Daskalakis V, Farantos S, Varotsis C ***Protein dynamics and spectroscopy for ferryl intermediate of Cytochrome c Oxidase: A molecular dynamics approach,*** International Conference of Computational Methods in Sciences and Engineering (**ICCMSE 2007**), *Corfu, Greece,* 2007. *(Award for Best Presentation, by the Organizing Committee of ICCMSE)*
Publication: ***Protein Dynamics and Spectroscopy for Ferryl Intermediate of Cytochrome c Oxidase: A Molecular Dynamics Approach***, ***AIP Computation in Modern Science and Engineering, Proc.*** 963(2): 31-34 (**2007**).

38. Pinakoulaki E, Ohta T, **Daskalakis V**, Aggelaki M, Kitagawa T, Ludwig B, Varotsis C **, ISBC2006**, Konan Fiber, Fiber, Konan University, Japan, 2006.

39. Daskalakis V, Frudakis G, Varotsis C ***DFT Study of endoperoxides and their intermediates in Fe(II) cleavage of the endoperoxy bridge,*** 19th National Conference in Chemistry, Heraklion, Crete, Greece, 2002.

ΔΙΚΤΥΑ ΚΑΙ ΣΥΝΔΡΟΜΕΣ ΜΕΛΟΥΣ

ΔΙΕΘΝΕΙΣ ΣΥΝΕΡΓΑΣΙΕΣ

Πρωτεΐνες Αίμης
Καθ. Βαρώτσης Κωνσταντίνος, Τμήμα Χημικών Μηχανικών, Τεχνολογικό Πανεπιστήμιο Κύπρου, Κύπρος
Καθ. Φαράντος Σταύρος, Τμήμα Χημείας, Πανεπιστήμιο Κρήτης & Ίδρυμα Τεχνολογίας Έρευνας, Ελλάδα
Prof. Teizo Kitagawa, Specially Appointed Professor; Graduate School of Life Science, University of Hyogo
Prof. Guallar Victor, ICREA Research Professor at Barcelona Supercomputing Center - Centro Nacional de Supercomputación (BSC-CNS). Life & Medical Sciences

Φωτοσύνθεση
Prof. Alexander Ruban, School of Biological and Chemical Sciences, Queen Mary, University of London
Prof. Ulrich Kleinekathöfer, Computational Physics and Biophysics Group, Jacobs University Bremen gGmbH, Department of Physics & Earth Sciences Focus Area Health
Dr. Christopher Duffy, Cellular and Molecular Biology, School of Biological and Chemical Sciences, Queen Mary, University of London
Prof. Kentaro Ifuku, Πανεπιστήμιο Κιότο, Ιαπωνία.

Θερμοσταθερότητα Πρωτεϊνών & Πρωτεΐνες Μη Σταθερής Δομής
Δρ. Κυριάκος Πετράτος, Ερευνητής, Εργαστήριο Κρυσταλλογραφίας ΙΙ, Ινστιτούτο Μοριακής Βιολογίας και Βιοτεχνολογίας, Ίδρυμα Τεχνολογίας Έρευνας, Ελλάδα (ITE)
Καθ. Κοτζαμπάσης Κυριάκος, Τμήμα Βιολογίας, Πανεπιστήμιο Κρήτης, Ελλάδα.
Αναπλ. Καθ. Παναγιώτης Μόσχου, Τμήμα Βιολογίας, Πανεπιστήμιο Κρήτης, Ελλάδα, Ίδρυμα Τεχνολογίας και Έρευνας (Ελλάδα), Πανεπιστήμιο Γεωπονικών Σπουδών (Σουηδία).

SARS-CoV-2
Καθ. Ηλίας Καστανάς, Ιατρική Σχολή, Πανεπιστήμιο Κρήτης, Ελλάδα
Καθ. Στέργιος Πυρίντσος, Τμήμα Βιολογίας, Πανεπιστήμιο Κρήτης, Ελλάδα

Πρωτεϊνες - Μεταφορείς
Καθ. Στάθης Φριλίγγος, Ιατρική Σχολή, Πανεπιστήμιο Ιωαννίνων

ΔΕΞΙΟΤΗΤΕΣ ΔΙΟΙΚΗΣΗΣ ΚΑΙ ΗΓΕΣΙΑΣ

Ακαδημαϊκή Καθοδήγηση

Πανεπιστήμιο Πατρών (2023 - σήμερα)

Διδακτορικές Εργασίες/ Υποψήφιοι Διδάκτορες (Ph.D):
Ενεργές (3): Θεοφάνη Ιωσηφίνα Σουσάνη, Boutheina Zender, Ηλίας Καρβούνης

Ερευνητικές Συνεργασίες:
Ενεργές (1): Πάνος Κούκος (μεταδιδακτορικός)
Ολοκληρωμένες (2): Αριάδνη Κωνσταντοπούλου (μεταδιδακτορικός), Κωνσταντίνος Χατζηκυριάκος (ερευνητικός συνεργάτης)

Προπτυχιακές Διπλωματικές Εργασίες (Πτυχίο Μηχανικού)
Ενεργές (6): Αναστασία Ιακώβου, Μινασιάν Αζάτ, Ναταλία Χρόνη, Καλλιόπη Καράντζη, Ναταλία Εμμανουηλίδη, Ανδρέας Γουσγουνέλλης
Ολοκληρωμένες (3): Τσίκλη Θεώνη, Τσιάβου Βαλεντίνα, Νίτας Παναγιώτης

Συμμετοχή στην Επιτροπή Αξιολόγησης Διδακτορικών Διατριβών:
1. Σωτήρης Ζερβέας (Πανεπιστήμιο Κρήτης, Τμήμα Βιολογίας)
2. Μαρία Πολυχρονάκη (Πανεπιστήμιο Κρήτης, Τμήμα Χημείας)
3. Χρήστος Κοσίνας (Πανεπιστήμιο Πατρών, Τμήμα Χημ. Μηχ.)
4. Αλέξανδρος Λυρατζάκης (Πανεπιστήμιο Κρήτης, Τμήμα Χημείας)
5. Δανάη-Μαρία Κοτζαμπάση (Πανεπιστήμιο Κρήτης, Τμήμα Βιολογίας)
6. Παναγιώτα Σιαχούλη (Ίδρυμα Τεχνολογίας και Έρευνας - Ελλάδα, ΙΤΕ)
7. Βασιλική Κ. Βαλαντή (Πανεπιστήμιο Κύπρου, Τμήμα Χημείας)

Τεχνολογικό Πανεπιστήμιο Κύπρου (2010 - 2023)

Προπτυχιακές Διπλωματικές Εργασίες (Πτυχίο)
Ολοκληρωμένες (9): Χαραλάμπους Φεβρωνία, Ιωάννου Νεοφύτα, Παναγιώτου Φωστήρα, Νεάρχου Ειρήνη, Δημητρίου Δ. Κωνσταντίνος, Γεωργίου Α. Γεωργία, Ελευθερίου Αντώνης, Βορκά Φλώρα, Χαραλάμπους Ανδρέας, Παλαζής Κ. Ανδρέας, Κατσώνη Παναγιώτα

Μεταπτυχιακές Διπλωματικές Εργασίες (δίπλωμα Master's)
Ολοκληρωμένες (5): Χαραλάμπους Φεβρωνία, Ιωάννου Νεοφύτα, Παπαδάτος Σωτήρης, Ανθή Χρυσαφούδη (σε συνεργασία με το Τμήμα Βιολογίας, Πανεπιστήμιο Κρήτης), Δανάη Μαρία Κοτζαμπάση (σε συνεργασία με την Ιατρική Σχολή του Πανεπιστημίου Κρήτης και το Ινστιτούτο Πληροφορικής του Ιδρύματος Έρευνας και Τεχνολογίας).

Διδακτορικές Εργασίες/ Υποψήφιοι Διδάκτορες (Ph.D):
Ολοκληρωμένες (1): Σαλάμεχ Αναστασία

ΑΚΑΔΗΜΑΙΚΑ ΚΑΙ ΔΙΟΙΚΗΤΙΚΑ ΚΑΘΗΚΟΝΤΑ

01/09/2023 – ΤΡΕΧΟΥΣΑ
Πανεπιστήμιο Πατρών

1. **Associate Editor**, Frontiers in Chemistry, Theoretical and Computational Chemistry section
2. Διακεκριμένο Μέλος της Αμερικανικής Ένωσης Χημείας (2024-2025)
3. Μέλος της **επιτροπής μεταπτυχιακών σπουδών του Τμήματος** Χημικών Μηχανικών (ΧΜ) του Πανεπιστημίου Πατρών (2024-2025)
4. Οργάνωση σεμιναρίων για την **επιλογή θεμάτων διπλωματικών εργασιών** στο πλαίσιο των προπτυχιακών σπουδών του Τμήματος ΧΜ (2024-2025).
5. Μέλος της **επιτροπής του κοινού προγράμματος στη Χημική Μηχανική με το Τεχνολογικό Πανεπιστήμιο Liaoning** (Liaoning University of Technology).

01/12/2010 – 31/08/2023
Τεχνολογικό Πανεπιστήμιο Κύπρου

1. **Μέλος του Συμβουλίου της Σχολής Γεωτεχνικών Επιστημών και Διαχείρισης Περιβάλλοντος** (2022-2023)
2. **Συγκλητική Επιτροπή Συστημάτων Πληροφορικής και Τεχνολογίας** (ΣΠΤ) (2012-2018)
(a) Αναθεωρήσεις του ετήσιου προϋπολογισμού του Πανεπιστημίου που αφορά την Υπηρεσία ΣΠΤ
(b) Επιτροπή του Έργου IdM (IAM) για την ενσωμάτωση του "Identity Access Management" στα πληροφοριακά συστήματα του Τεχνολογικό Πανεπιστήμιο Κύπρου
(c) Επιτροπή για το Έργο «Λογισμικά Microsoft για φοιτητές»

(d) Επιτροπή για την πολιτική και τους κανόνες πρόσβασης στο διαδίκτυο από τους χρήστες του Τεχνολογικού Πανεπιστημίου Κύπρου
3. **Επιτροπή Προπτυχιακών & Μεταπτυχιακών Σπουδών** του Τμήματος (2011-2023)
4. **Επιτροπή Διασφάλισης Ποιότητας του Τμήματος** (2011-2018)
5. Την Ad hoc Επιτροπή Μονάδων ECTS του Τεχνολογικού Πανεπιστημίου Κύπρου (2014)
6. Την Ad hoc Επιτροπή για το «Ανοιχτό Πανεπιστήμιο» (2016-2023)
7. Την Επιτροπή Παγκύπριων Εξετάσεων για την εισαγωγή στην Ανώτερη Εκπαίδευση Κύπρου-Ελλάδας (2014)
8. Μέλος της εφορευτικής επιτροπής για την εκλογή των Ακαδημαϊκών μελών του Συμβουλίου του Πανεπιστημίου (2012)
9. Μέλος της επιτροπής RAC για κατανομή υπολογιστικού χρόνου στο Cyclone (Ινστιτουτο Κύπρου)

ΕΚΠΑΙΔΕΥΤΙΚΟ ΕΡΓΟ

Ανεξάρτηση Διδασκαλία

Πανεπιστήμιο Πατρών, Τμήμα Χημικών Μηχανικών (Προπτυχιακά):
(1) CHM-163 Εργαστήριο Υπολογιστών (Χειμερινά Εξάμηνα 2023-2025), (2) CHM-363 Εισαγωγή στον Προγραμματισμό - Θεωρία & Εργαστήριο (Χειμερινά
εξάμηνα 2023-2025)
Πανεπιστήμιο Πατρών, Ιατρική Σχολή (Μεταπτυχιακά):
(1) Μεθοδολογία στην Έρευνα Βιοεπιστημών BIE - Προσομοιώσεις Βιομοριακών αλληλεπιδράσεων (2023-2024)
Πανεπιστήμιο Ιωαννίνων, Ιατρική Σχολή (Μεταπτυχιακά):
(1) Λειτουργική Ανάλυση Γονιδίων: Από τον Σχεδιασμό στο Έμβιο Σύστημα - Βιομοριακές Προσομοιώσεις και ορθολογικός σχεδιασμός φαρμάκων (2024-2025)
Πανεπιστήμιο Κρήτης, Τμήμα Βιολογίας (Μεταπτυχιακά):
«ΦΩΤΟΣΥΝΘΕΣΗ: Η φωτοσυνθετική μηχανή στο μικροσκόπιο της Μοριακής Δυναμικής», στο μεταπτυχιακό πρόγραμμα «Μοριακή και Εφαρμοσμένη Βιολογία Φυτών – Πράσινη Βιοτεχνολογία» (Χειμερινο Εξάμηνο 2023/ Εαρινά Εξάμηνα 2019-2022)
Πανεπιστήμιο Κρήτης, Ιατρική Σχολή (Μεταπτυχιακά):
«Στο μικροσκόπιο της Μοριακής Δυναμικής», στο μεταπτυχιακό πρόγραμμα «Βιοπληροφορική» (Φθινοπωρινό Εξάμηνο 2021)

Τεχνολογικό Πανεπιστήμιο Κύπρου (Μεταπτυχιακά):
(1) Υπολογιστική Περιβαλλοντική Χημεία, Βιοχημεία και Βιολογία (Εαρινά εξάμηνα 2012-2017), (2) Ειδικά Θέματα στην Περιβαλλοντική Βιοεπιστήμη (Φθινοπωρινό εξάμηνο 2014)
Τεχνολογικό Πανεπιστήμιο Κύπρου (Προπτυχιακά):
(3) Υπολογιστικά Περιβαλλοντικά Μοντέλα & Εισαγωγή στο MATLAB (Εαρινά εξάμηνα 2011-2020) (4) Μοντέλα Διασποράς (Φθινοπωρινά εξάμηνα 2011-2020), (5) Φυσική Περιβάλλοντος (Φθινοπωρινό εξάμηνο 2011), (6) Αρχές Θερμοδυναμικής & Χημικής Κινητικής (Εαρινά εξάμηνα 2011-2012), (7) Εφαρμοσμένη Θερμοδυναμική ΙΙ (Εαρινά Εξάμηνα 2020-2022), (8) Δυναμική Προσομοίωση Συστημάτων με τη βοήθεια Η/Υ (Φθινοπωρινά εξάμηνα 2019-2022), (9) Μαθηματικά ΙΙΙ (Διαφορικές Εξισώσεις) (Φθινοπωρινά Εξάμηνα 2021-2022), και (10) Φυσική ΙΙ (Ηλεκτρισμός - Μαγνητισμός - Ηλεκτρομαγνητισμός) (Εαρινό Εξάμηνο 2022).

ΔΙΔΑΣΚΑΛΙΑ:
Ενδεικτική λίστα μαθημάτων που μπορώ να διδάξω ανεξάρτητα: Γενική Χημεία, Βιοχημεία Ι-ΙΙ, Βιο-Μαθηματικά, Φυσικοχημεία – Θερμοδυναμική, Φασματοσκοπία, Βιοστατιστική, Υπολογιστική Βιολογία, Δομική Βιολογία, Προγραμματισμός, Δομή και Λειτουργία Πρωτεϊνών, Προσομοίωση Βιολογικών Συστημάτων: μέθοδοι πρόβλεψης δομής.