



Vangelis Daskalakis

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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

01/09/2023 – CURRENT Patras, Greece

ASSISTANT PROFESSOR DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS

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

Research Grants:

- 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**).
- 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**
- Cyclone 2022A Production Access: **pro22a103s1** - "*Fucoxanthin - chlorophyll protein (FCP): from monomers to tetramers*", **150.000 GLU-core hrs** on Cyclone.
- Proposal No. EHPC-REG-2023R01-128 **EuroHPC Regular Access Call "Peptaibols: How to kill a bacterium"**, **6.400.000 CPU-core hrs** on MeluXina.

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

01/05/2022 – 31/08/2023 Limassol, Cyprus

ASSOCIATE PROFESSOR DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY

Research/ Grants:

- 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**).
- Erasmus+ Learning Mobility of Individuals – Staff mobility for teaching and training activities, Queen Mary University of London (**May 2022**)

31/12/2014 – 30/04/2022 Limassol, Cyprus

ASSISTANT PROFESSOR DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY

Research/ Grants:

- 13th Allocation **Cyclone (The Cyprus Institute)** project CfP13 - "*Molecular Dynamics of LHCI 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 LHCPSalt** "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, Ispre400, Ispre410, **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.

30/11/2010 – 30/12/2014 Limassol, Cyprus

LECTURER DEPARTMENT OF CHEMICAL ENGINEERING, CYPRUS UNIVERSITY OF TECHNOLOGY

Research/ Grants:

1. Startup Grant Cyprus University of Technology (40.000 €)
2. "Activation and reduction of Nitric Oxide (NO) to laughing gas (N₂O) 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 Isprob104s1, Ispro13a121s1, 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).

Barcelona, Spain

VISITING POSTDOC LIFE SCIENCES DEPARTMENT, BARCELONA SUPERCOMPUTING CENTER

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

2006 – 2010 Heraklion, Crete, Greece

RESEARCH COLLABORATOR INSTITUTE OF ELECTRONIC STRUCTURE AND LASER OF THE FOUNDATION FOR RESEARCH AND TECHNOLOGY HELLAS

GRID COMPUTATIONAL CHEMISTRY – GRID-COMP-CHEM – 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, 3^d and 4th year IKY Scholarship for Excellence (1996-2000), (3) 3^d 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 revealed by Density Functional Theory and *resonance* Raman".

Ph.D Title: "Bioenergetic Mechanisms of O₂ 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 O₂ 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 reductase (nor)

Financial entity: **Greek Ministry of Education, General Secretariat for Scientific Research (2000-2001)**

Address Voutes, Hraklion, 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

● ADDITIONAL INFORMATION

BRIEF SUMMARY OF RESEARCH INTERESTS

Research Outcome

47 publications as articles in **peer-reviewed journals (40)**, **book chapters (6)** and **conference proceedings (1)**. **First author in 20/47** and the **corresponding author in 21/47** publications, exerting strong independence (h-index Scopus 15, Google Scholar 16). 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 Sci. Rep., J. Phys. Chem. B-C, 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 (**180 Reviews for Journals**, Web of Science – publons). 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). **39 participations in International Conferences - Seminars**, including **11** invited lectures. My research is featured in the **PRACE DIGEST 2017, 2020** from *Insight Publishers*.

The lab - Research Focus

My independent research focuses on the biophysics of large biological and small gaseous molecules involved in processes related to life sciences (Biology, Biomolecular Engineering) and/ or the environment. In the lab we employ elaborate computational techniques based on the Molecular Dynamics (MD) method (like the 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 PRACE/ DECI (<https://prace-ri.eu/>) schemes (Joliot Curie - Irene ROME TGCC in Bruyères-le-Châtel, Salomon i4i 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.

(A) Heme proteins

Heme proteins (19 publications), and especially the interaction of myoglobin (Mb) and Cytochrome c Oxidase (CcO) with atmospheric gases (O_2 , COx, NOx), or the dynamics of cytochromes in drug metabolism. Insight into their in vivo behavior and possible environmental sensor capabilities has been obtained. The research outcomes, for the heme proteins, are summarized in the following. Nitrite is a powerful oxidizing agent and a biological reservoir for NO that has been implicated in a variety of aerobic biological systems. The “greening” process in the reaction of ferric Mb with NO_2^- proceeds through the Fe-O-N=O/2- nitrovinyl species. We have shown that the coordination or removal of NO_2^- to/from the heme iron is associated mainly with a motion of helix E and the coordination of NO_2^- to the 2-vinyl is associated with a motion of helix F and a correlated motion of helices E-F. This latter correlated motion has been attributed to the interaction of Val68 and Ile107 with the 2-nitrovinyl moiety. On the other hand, Nitric oxide reductase (NOR) is the third of the four enzymes of bacterial denitrification responsible for the catalytic formation of laughing gas (N_2O). We have reported the detection of the hyponitrite ($HO-N=N-O^-$) species ($\nu_{N-N} = 1332\text{ cm}^{-1}$) in the heme b_3 Fe-Fe_B dinuclear center of NOR from *Paracoccus denitrificans*. Finally, the identification of the intermediates and determination of their structures in the reduction of dioxygen to water by cytochrome c oxidase (CcO) are particularly important to understanding both O_2 activation and proton pumping by the enzyme. We have recently proposed that the environment proximal to the heme a_3 controls the spectroscopic properties of the ferryl intermediates in cytochrome oxidases.

(B) Photosystem II Light Harvesting Complexes

Photosystem II Light Harvesting Complexes (13 publications), and especially the mechanism of excess energy dissipation (Non-Photochemical Quenching or NPQ); the photoprotective mechanism in higher plants and algae that is highly relevant to a changing climate in terms of the production of tolerant plants, the O_2 evolution, the CO_2 fixation and the increased crop production. Photosynthesis and Photosystem-II inspired models can potentially lead to applications in artificial and more efficient solar energy harvesting. It can also be related, in a timely manner, with the engineering of tolerant plants in a changing planetary climate (light stress, heat waves, increase of salinity in a deteriorating water quality). However, the drawback for an efficient photosynthetic process or increased crop yields, lies in the fact that under excess light conditions, organisms activate their photoprotection and convert a significant amount of photonic energy into heat. Atomic scale insight into this mechanism is lacking in the literature. Transitions between protein states are triggered by external stimuli. This knowledge leads to the control of protein function. We have reported so far, a large scale (150 μ s) study on the conformational space of the major Light Harvesting Complex II (LHCII), based on a comprehensive array of external stimuli. Our LHCII models at \AA -atom resolution have provided the complete computational framework to drive the LHCII conformation between, previously elusive, different states, associated with light harvesting and quenched modes. Thus, we have probed for the first and at the same time the effects of all the key NPQ factors, on the LHCII trimer conformation. Even with the extensive sampling reported in our studies, for the LHCII scaffold transitions, a hard switch between light harvesting and quenching is still absent in the induced inter-pigment (Chlorophyll – Carotenoid) interactions.

Thus, our studies have shifted the attention from the extensive conformational sampling, to the problem of accurately describing inter-pigment interactions within LHCII (i.e. by accurate ab initio methods).

(C) SARS-CoV-2 proteins

SARS-CoV-2 proteins (3 publications), and especially the dynamics of the main protease (MPro) and the nucleocapsid protein (NC). It is well established that the conformation of a protein in a crystal is usually far from the in-vivo conformation which is relevant for pharmacology. MD methodology is an ideal tool for this purpose, and we managed to drive the rigid protein in crystals towards in-vivo conformations, relevant to target the COVID-19 disease. We identified two natural products that might facilitate: (a) weakening of the main protease dimerization, and (b) weakening of the nucleocapsid – importins interactions. Importins *are a type of karyopherins that transport protein molecules from the cell's cytoplasm to the nucleus. This is crucial for the replication of the virus, as its genetic material must reach the host cell nucleus to employ the host replication machinery.*

(D) Thermostability of proteins

Thermostability of proteins (2 publication) and especially that of a cold-adapted alcohol dehydrogenase. We have provided the dynamics of the protein under extreme conditions of temperature to supplement the structure of a recombinant (His-tagged at C-terminus) alcohol dehydrogenase (MoADH) from the cold-adapted bacterium *Moraxella* sp. TAE123 that was refined with X-ray diffraction data extending to 1.9 Å resolution. MD simulations showed enhanced wide-ranging mobility of MoADH at high temperatures. Principal component analysis of the fluctuations resulted in a prominent open–close transition of the structural domains mainly at 280 K for MoADH.

(E) Studies on water dynamics

Studies on water dynamics (salt – organic hydration) (4 publications), viewed from the physical chemistry aspect, add to the multi-disciplinary nature of my research and are used in current projects as the biomimetic membranes for water desalination systems, but also as the basis for protein-hydration dynamics.

(F) The CRISPR-Cas9 system

The CRISPR-Cas9 system (2 publications) edits genes by cleavage of a specific target DNA sequence within, and then letting natural DNA repair processes to take over. The system consists of two parts: the Cas9 enzyme and a guide RNA complementary to the target DNA sequence. We aim at improving the specificity of the system and reducing the Cas9 enzyme size for efficient delivery.

PROJECTS

2014 – CURRENT

Dynamics of the Light Harvesting Complexes of Photosystem II

2017 – CURRENT

Thermostability of Proteins at extremes

04/2020 – CURRENT

Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution

2017 – CURRENT

Water desalination based on bio-mimetic membranes

1999 – CURRENT

Heme proteins

2021 – CURRENT

The CRISPR-Cas9 system

PUBLICATIONS

01. 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

02. Recognition motifs for Importin 4 [(L)PPRS(G/P)P] and Importin 5 [KP(K/Y)LV] binding, 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

03. 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/acspchemau.2c00041

04. 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.

05. 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

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

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

07. 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

08. 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

09. 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

10. 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

11. 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

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

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

13. 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

14. 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

15. On a Chlorophyll-Carotenoid Coupling in LHCII

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

16. 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

17. The Photosystem II Subunit S under Stress

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

18. 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.

19. 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.

20. 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.

21. Nitrite coordination in myoglobin

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

22. Energizing the Light Harvesting Antenna: Insight from CP29

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

23. 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

24. 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.

25. 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.

26. 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.

27. 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.

28. 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.

29. 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.

30. 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.

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

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

32. 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

33. 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

34. 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

35. 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

36. 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

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

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

38. 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

39. 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, Stavarakis S, Marialena A, Papadopoulos G, **Daskalakis V**, Varotsis C* (2005) *J. Raman Spec.* 36: 337-349

40. 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, Stavarakis S, **Daskalakis V**, Varotsis C* (2004) *Bioch. Biophys. Acta* 1655: 347-352

REVIEW ARTICLES/ BOOK CHAPTERS-----

41. 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.

42. 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

43. 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

44. 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

45. 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

47. 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

46. 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

CONFERENCES AND SEMINARS

2023

Conferences - Seminars - Workshops 1. Daskalakis V. "Biomolecular Engineering: Structures and Dynamics". Seminar at the Department of Physics, Constructor University, Bremen, Germany, 27 April 2023 (*invited talk*)

2. 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*)

3. 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 LHCI 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. 62nd 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.** 3^d 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: Implications 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 a₃ 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, Institut 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 Cellular 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 + O₂ 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 + O₂ 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

Protein Thermostability - IDPs

Dr. Kyriacos Petratos, Principal Researcher, Laboratory of Crystallography, Institute of Molecular Biology and Biotechnology, Foundation for Research and Technology Hellas (FORTH).

Prof. Kotzabasis Kiriakos, Dept. Biology, University of Crete, Greece

SARS-CoV-2 Targets

Prof. Elias Castanas, School of Medicine, University of Crete

Prof. Stergios Pirintsos, Dept. Biology, University of Crete, Greece

ACADEMIC & ADMINISTRATIVE DUTIES

Cyprus University of Technology

1. Member of the **General Assembly of the Faculty** of Geotechnical Sciences and Environmental Management (2022-present)
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-present) & **Undergraduate Committees** (2017-present)
4. The Departmental **Committee on Quality Assurance** (2011-present)
5. The *Ad hoc* **ECTS label Committee** of the Cyprus University of Technology (2014)
6. The *Ad hoc* **committee for the Open University** (2016-present)
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

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)

University of Crete, Department of Biology (visiting): «**Photosynthesis: The Photosynthetic apparatus under the microscope of Molecular Dynamics**», in postgraduate program «Molecular and Applied Plant Biology – Green Biotechnology» (Spring Semesters 2019-2022)

University of Crete, School of Medicine (visiting): «**Under the Microscope of Molecular Dynamics**», in postgraduate program «Bioinformatics» (Autumn Semester 2021)

Cyprus University of Technology Undergraduate: (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

MANAGEMENT AND LEADERSHIP SKILLS

Student Mentoring 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 (Cyprus University of Technology)

Postgraduate Diploma Theses (Master's degree)

Completed (5): Charalambous Fevronia, Ioannou Neofyta, Papadatos Sotirios (Cyprus University of Technology), 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 (Cyprus University of Technology)

Participation in Examiner's Board for diploma theses (under/post-graduate): 24