2022 Final Project Report

for

Academic Consortium for the 21st Century (AC21)

Special Project Fund

Towards healthy aging by antioxidants: from molecular mechanism to cellular function

Project Group Leader: Prof. Dr. Yachong Guo

Nanjing University

Date of Activities: March 2022 – February 2023

Project Abstract

Aging is a process characterized by the progressive loss of tissue and organ function, reactive oxygen and nitrogen species are produced by several endo/exogenous processes, and play a significant role in aging as well as in age-related diseases. Although the free radical theory of aging has been widely accepted among scientists, it is particularly challenging to apply antioxidants to delay the aging processes-motivating the research towards basic physical chemistry and biological behavior of oxidative stress, antioxidants, and the complex interactions between them. In order to bridge the gap between molecular mechanisms and cellular function, provide solid foundation for the application of antioxidants, we put the resources and skills of AC21 members around the world together.

By cooperatively planning the research activities, the project aims to strengthen the communication and bring together different groups, create opportunities for junior researchers, initialize the potential fund for long term research projects and bridge the gap between the physical/chemical mechanisms and the cellular functions of antioxidants, eventually benefit health of human being and achieve funding success. The project anticipates a wide-ranging impact in the fields of research, education, management and international exchanges. This project also promised to provide an important contribution to the research cooperation of the university or environment and contribution to the development of the individual participants and further strengthen the AC21 network.

Activities and Reports

Mar. 2022	• Early stage discussion for the project and student exchange plan. • Discussion between PIs about the initial research plan, collaboration between researchers, including graduate students. • Discussion the potentials between colleges to advance the exchange between undergraduate student to strength the collaboration.
Apr. 2022	• Student exchange between France and Germany. (Short term within 3 months) • Discuss the potential research funding between France/Germany and China (e.g. Sino-German project); France and Germany (e.g. DAAD project, EU project). • Shared Lab seminars between groups.
May – June 2022	• Student's exchange between EU and China. (Long term between 3-6 months). • Meet at France, Strasbourg of PIs and selected students for onsite discussion, advance the administration of undergraduate student exchange and future collaboration. • Early discuss and advisement (website creation) about the workshop in Nanjing China.
July 2022	• Preparation of the progress report between PIs. Evaluate and discuss the Short-term student exchange outcome, prepare the research article and scientific report.
Aug. 2022	• Plan the details of the international workshop in Nanjing, China.
Sep. – Oct. 2022	• Evaluate and discuss the Long-term student exchange outcome (one month ahead), prepare the research article and scientific report. Hold an international workshop in Nanjing, China. • Hold an international workshop in Nanjing, China.
Nov. 2022	• Evaluate and discuss the outcome and improvement of the international workshop in Nanjing, China. Strengthen the collaboration of the potential partners and research collaborations from thethe project.
Dec. 2022 – Feb. 2023	• Students exchange progress discussion. • Evaluate and discuss the outcome of the discussion, newsletter, and technical papers. • Prepare the article for AC21 newsletter. • Final project report. • Final financial report.

Achievement of Activities

Nanjing University, University of Strasbourg, and University of Freiburg have long strategic partnership and relationship, employing complementary advantages and interdisciplinary scholarships to promote research cooperation and academic exchange. This project aims to strengthen the communication and bring together different groups, create opportunities for junior researchers, initialize the potential fund for long term research projects and bridge the gap between the physical/chemical mechanisms and the cellular functions of antioxidants, eventually benefit health of human being and achieve funding success.

Research:

This project combined theoretical and experimental methods to explore the mechanism and application of aging-related antioxidants. We sought to bridge the gap between the physical/chemical mechanisms and the cellular functions of antioxidants by the combination and promotion of Nanjing University's theory and simulation, experiments and application of University of Strasbourg and University of Freiburg, leading to the substantive engagement of researchers in the areas of interdisciplinary study.

Education:

The research solutions are incorporated with multiple disciplines of physics, chemistry and life science courses both at undergraduate and graduate levels within the Kuang Yaming Honors School, offering the cutting-edge courses of the interdisciplinary sciences. The exchange of graduate/undergraduate students and advance interdisciplinary courses both in theory and experiments will facilitate students' research skills and later strengthen by assigning research programs.

International Exchange:

By developing the visiting/exchange of graduate/undergraduate student between universities. This project is promised to provide an important contribution to the research cooperation of the university or environment and contribution to the development of the individual participants and further strengthen the AC21 network.

Achievements made with SPF collaboration

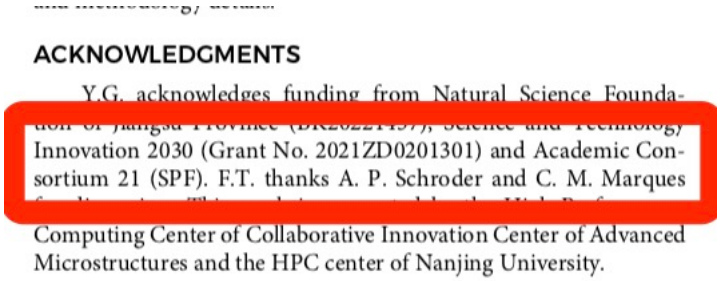
From the moment of receiving the budget. We have immediately managed the Early-stage discussion for the project and student exchange plan, initial research plan, collaboration between researchers, including graduate students. Due to the circuit breaker of flights to China, restrict the activities between Nanjing University is organized online. The online lab seminars between PI and students between all partners are organized every week. 3 PhD students 2 master students constantly joined the seminar focusing on the project of physical/chemical mechanisms and the cellular functions of antioxidants. Poster presentation are held at the KMF Summer Scientific Training, 6-8 July 2022, Nanjing, P.R.China.

We have invited in total 12 distinguished researchers in the biology, physics, chemistry are of antioxidants to give online seminar focusing of the molecular mechanisms and cellular function of oxidants. We published several peer-reviewed articles on distinguished journals focusing on the molecular mechanisms and application of antioxidants in acknowledge of AC21. Our work taking into account the molecular mechanisms and cellular function of oxidants, especially in the drug design aspect catches attention of Nobel Prize winner Prof. Jean-Marie Lehn (1987 Nobel Prize in Chemistry, Strasbourg University). He joined our network and gives high expectation to our future collaboration and work we have done.

Due to the covid, the originally planned offline communication didn't proceed smoothly, but we used the online form to communicate with various organizations, successfully gathered different groups, created opportunities for junior researchers. Prof. Fabrice and Prof. Yachong initiated long-term research projects from joint EU-NSFC fund, aiming to bridge the gap between physical/chemical mechanisms and cells, and the function of antioxidants, which ultimately contributed to human health and achieved the success of the fund. By the SPF support from AC21, we expect to have a broad impact in research, education, management and international exchanges.

Photos & link(s)

Zhang, Yangyang, Donghui Liu, Yiyang Zhang, **Yachong Guo**, Wenfei Li, and **Fabrice Thalmann**. "Coarse-grained description of monounsaturated peroxidized phospholipid bilayers." The Journal of Chemical Physics 157, no. 8 (2022): 085103.
https://aip.scitation.org/doi/10.1063/5.0096658?af=R



ACKNOWLEDGMENTS

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Computing Center of Collaborative Innovation Center of Advanced Microstructures and the HPC center of Nanjing University.

Yachong, Guo, Marco Werner, and **Vladimir A. Baulin**. "Efficient enumeration-selection computational strategy for adaptive chemistry." Scientific reports 12, no. 1 (2022): 1-13.
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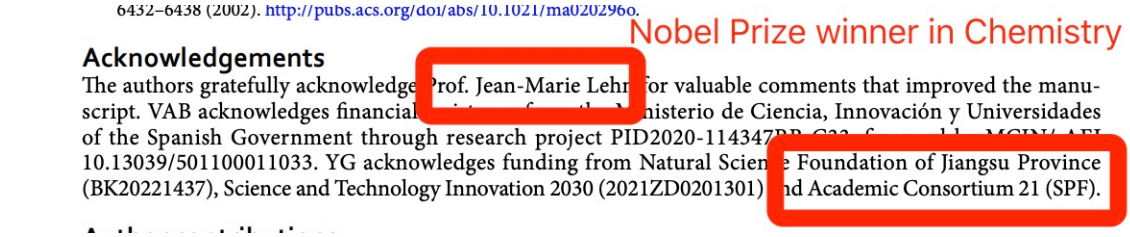

6432–6438 (2002). http://pubs.acs.org/doi/abs/10.1021/ma0202960.

Nobel Prize winner in Chemistry

Acknowledgements

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(bold name is the network member)

Selected international online forum

2022 Academic Reports

Towards healthy aging by antioxidants: from molecular mechanism to cellular function

Prof. Dr. Yachong Guo

Kuang Yaming Honors School, Nanjing University

Resume: Professor of Kuang Yaming College of Nanjing University, Institute of Brain Sciences of Nanjing University, supervisor of Biomedical Physics Laboratory of Nanjing University, lifelong visiting professor of Leibniz Polymer Institute of Germany and Dresden University of Technology. The research direction is the intersection of soft condensed matter physics, chemistry and biological science.

Abstract: We will explore how to understand life phenomena and even predict new life phenomena from the basic principles of physics, and connect micro, meso and macro with basic physical principles from the molecular level to the cell level. For biological aging, it is a process characterized by the progressive loss of tissue and organ function, reactive oxygen and nitrogen species are produced by several endo/exogenous processes, and play a significant role in aging as well as in age-related diseases. Although the free radical theory of aging has been widely accepted among scientists, it is particularly challenging to apply antioxidants to delay the aging processes-motivating the research towards basic physical chemistry and biological behavior of oxidative stress, antioxidants, and the complex interactions between them.

Dec. 05. 2022 16:00 - 19:00

Tencent Meeting: 571-290-425

2022 Academic Reports

AIMD computational simulation study of radiation biological effects

Prof. Dr. Bin Gu

School of Physics and Optoelectronic Engineering, Nanjing University of Information Science and Technology

Resume: Graduated from Beijing Normal University in 2008, majoring in Particle Physics and Nuclear Physics, with a Ph.D. Then he worked in Nanjing University of Information Science and Technology. From 2018 to 2021, he was the Research Fellow of the EU Horizon 2020 innovation program "Enable Smart computation for Space Radiation" project, and carry out multi-scale simulation research on ion radiation damage effects. He has published more than 40 papers in Phys Rev Lett, J Phys Chem, Rad Chem Phys and other journals.

Abstract: Research on the biological effects of ion radiation from the sub-molecule scale can provide an important theoretical basis for the development of manned aviation, medical physics and other fields. The speaker will introduce his and his collaborators' research on the physical mechanism of DNA damage caused by secondary low-energy electrons in the process of ion radiation using the AIMD simulation method, as well as the efficient ab initio calculation of biological media on the electron energy loss of the ion beam in the Bragg peak region.

Nov. 28. 2022 16:00 - 19:00

Tencent Meeting:571-290-425