

# AUGUST - SEPTEMBER 2020 ISSUE 14

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### Prof. Li Xuehua Published Her Latest Work in EHP

Source: School of Environmental Science and Technology

The team of Associate Professor Li Xuehua from School of Environmental Science and Technology at DUT, and the team of Professor Li Ruibin from Soochow University have collaborated in the field of international environmental health and published an article entitled "Quantitative structure-activity relationship models for predicting inflammatory potential of metal oxide nanoparticles" (DOI:10.1289/EHP6508) in *Environmental Health Perspectives*, which is an international authoritative journal (https://ehp.niehs.nih.gov/doi/10.1289/EHP6508). This study constructed the first machine learning model to achieve the prediction of the inflammatory effect of nano-

materials causing lung fibrosis. It not only provides an important tool for risk evaluation of nanomaterials, but also expands the understanding of the mechanism of the inflammatory effect of nanomaterials.

Although substantial concerns about the inflammatory effects of engineered nanomaterial (ENM) have been raised, experimentally assessing toxicity of various ENMs is challenging and time-consuming. Alternatively, quantitative structure—activity relationship (QSAR) models have been employed to assess nanosafety. However, no previous attempt has been made to predict the inflammatory potential of ENMs.

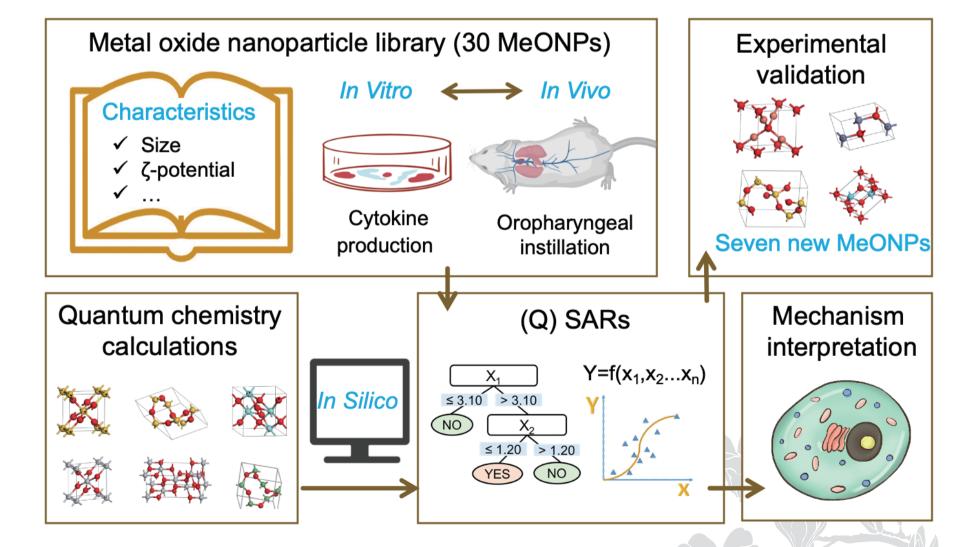


Figure 1. Schematic workflow of metal oxide nanomaterials (MeONPs) library construction, predictive modeling, mechanism interpretation, and experimental validation.

By employing metal oxide nanoparticles (MeONPs) as a model ENM, they aimed to develop QSAR models for prediction of the inflammatory potential by their physicochemical properties. They built a comprehensive data set of 30 MeONPs to screen several pro-inflammatory cytokines in THP-1 cell line. A pro-inflammatory cytokine of IL-1β could be used as an index to rank the inflammatory potential of MeONPs. Seventeen out of 30 MeONPs induced excess IL-1β production in THP-1 cells. The in vitro hazard ranking was validated in mouse lungs by oropharyngeal instillation of six randomly selected MeONPs.

In vivo disease outcomes were highly relevant to the in vitro data. They established QSAR models for prediction of MeONP-induced inflammation via machine learning, with predictive accuracy (ACC) exceeding 90%. The models were further validated experimentally against seven independent MeONPs (ACC=86%). Density functional theory (DFT) computations and experimental results further revealed that the key mechanisms driving inflammatory responses of MeONPs were proton sponge effect, cellular internalization, lysosomal damage, and release of toxic ions.

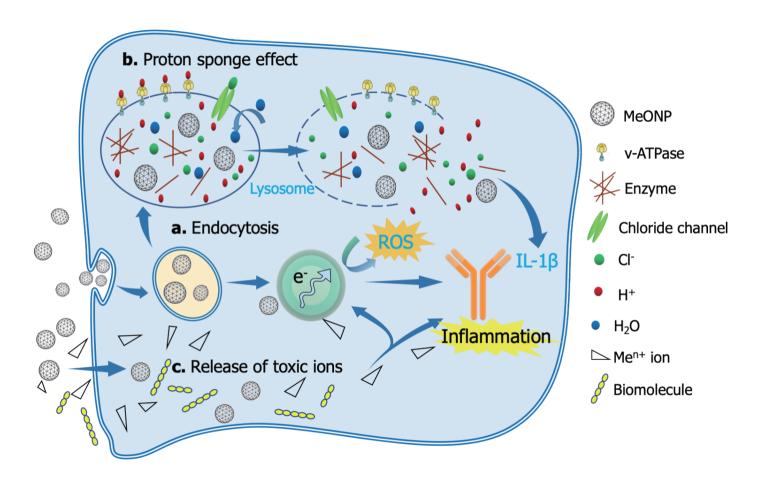


Figure 2. Proposed schematic image of inflammatory mechanisms by metal oxide nanomaterials (MeONPs). (A) Endocytosis: MeONPs with a positive  $\zeta$ -potential were most internalized by THP-1 cells and lysosomes. (B) Proton sponge effect. MeONPs with metal atom electronegativity  $\leq 1.55$  tend to trigger a proton sponge effect, followed by lysosome damages, leakage of lysosomal contents and excess IL-1 $\beta$  production. (C) Release of toxic ions.

Environmental Health Perspectives (EHP) is a monthly international authoritative journal of environmental health research and news. Retrieved by Web of Science, the journal has published 174 papers in 2019, with a total of 15 papers from the first completion unit in China.

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# **New Publication from DUT in Nature Communications**

Source: School of Economics and Management

nature > nature communications > articles > article



# nature communications

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Article | Open Access | Published: 05 June 2020

# Modular gateway-ness connectivity and structural core organization in maritime network science

Mengqiao Xu $\stackrel{igsq}{\sim}$ , Qian Pan, Alessandro Muscoloni, Haoxiang Xia $\stackrel{igsq}{\sim}$ & Carlo Vittorio Cannistraci $\stackrel{igsq}{\sim}$ 

Nature Communications 11, Article number: 2849 (2020) | Cite this article

Professor Xia Haoxiang's team from the School of Economics and Management and the Research Center for Big Data and Intelligent Decision-Making of DUT recently published their work entitled "Modular gateway-ness connectivity and structural core organization in maritime network science" (https://www.nature.com/articles/s41467-020-16619-5) in *Nature Communications* in collaboration with Dr. Carlo Cannistraci's team from Dresden University of Technology, reporting their findings on the structural characteristics of the global liner shipping network.

It is of great importance to establish the better understanding on the maritime transportation system for both academia and policy-making, since around 80% of global trade by volume is transported by sea, and thus the maritime transportation system is fundamental to the world economy. To this end,

the two teams collaboratively investigated the structural properties of the global liner shipping network (GLSN), finding that it is an economic small-world network with a trade-off between high transportation efficiency and low wiring cost. Furthermore, the mode of local segregation and global integration was examined by using three respective structural measures. In particular, with a new gateway-hub measure being introduced, their work reveals a distinctive structural-core structure of the investigated network that endogenously evolves into the backbone of the global maritime cargo transportation system. This finding offers new insights into the GLSN's structural organization complexity and its relevance to the international trade. From network science point of view, this investigation also sheds light on the efficient and robust organization of real-world complex networks.

Nature Communications, as a Nature-branded academic journal under Springer Nature Publishing Group, is one of the leading journals on multidisciplinary sciences. It publishes high-quality researches across all areas of natural sciences and quantitative social sciences. In the latest release of Clarivate Inc.'s JCR Report of Web of Science, its impact factor is 11.878, ranked the fifth in the category of multidisciplinary-science journals.

This work was co-directed by Prof. Xia and Dr. Cannistraci. Prof. Xia's research team initiated the overall research project and developed the key concept of segregation-integration in the context of the global liner shipping network. Dr. Cannistraci's team played a critical role in analyzing the GLSN in the hyperbolic space, as an important technical part of the paper. Dr. Xu Mengqiao, post-doc at Prof. Xia's group, suggested the gateway-hubness measure for the GLSN, while PhD student Pan Qian, also from Xia's group, did a great part of research in the computational data analytics on the network properties. The research was supported by the National Natural Science Foundation of China under Grants Nos. 71871042, 71533001, and 71421001, respectively.

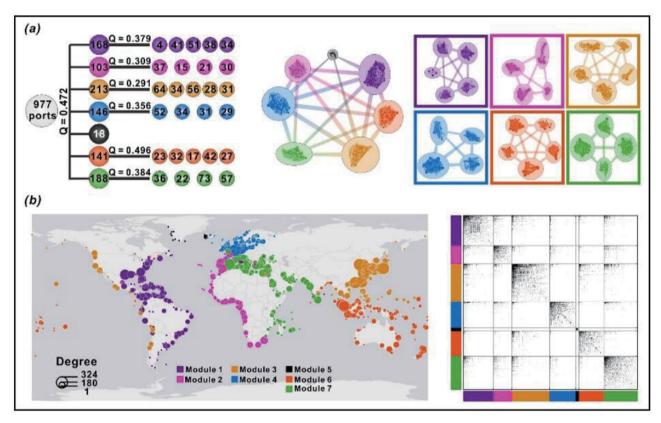


Figure 1. Multiscale modular communities in the GLSN.

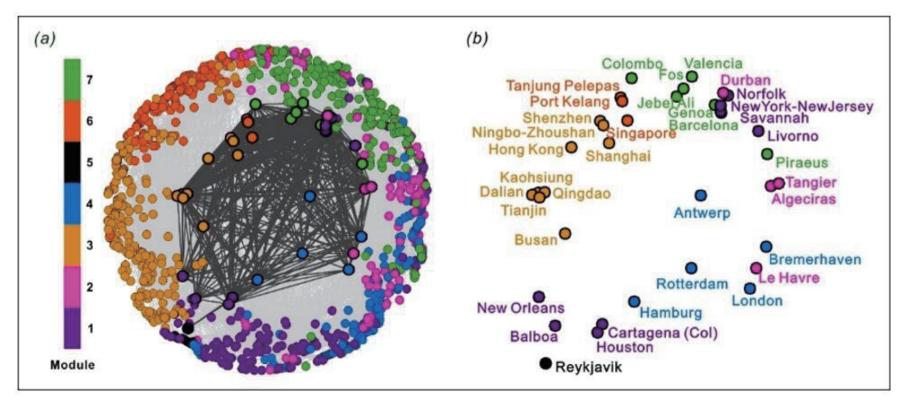


Figure 2. Representation of the GLSN and its structural core in the hyperbolic space.

# DLI Student Awarded Raymond Peacock Prize by UoL

#### Source: Leicester International Institute, DUT

Recently, good news traveled from the University of Leicester that Shan Xufeng, who is a student of Leicester International Institute, Dalian University of Technology, and now studying at the University of Leicester via the 2+2 transfer program since September 2019, was awarded the Raymond Peacock Prize.

The Raymond Peacock Prize is an endowed prize from Professor Raymond Peacock, who was Professor of Inorganic Chemistry in the School of Chemistry from 1965 until 1991. The Prize is awarded annually to the best 2nd year student.

Shan Xufeng is a student of 2017 Class majoring in Chemistry programme. Before he transferred to the UK, he was dedicated himself to study at Dalian University of Technology, and was awarded the scholarships for outstanding academic achievement for both the 2017-2018



academic year and 2018-2019 academic year. After two years' study at the Sino-British joint educational institute with the deeply integrated educational ideas, various measures of English training and the combination of Chinese and British education, even under the strict requirements and new challenges, Shan Xufeng has quickly adapted to the British teaching method and learning environment in the UK. After a year of hard study, he has got the highest marks at the School of Chemistry.

With the persistent principle of mutual integration of educational ideas, cultural intercommunication, resource sharing and win-win cooperation, DLI has built up the internationalised teaching model to achieve the same standard of education as both Dalian University of Technology and the University of Leicester. DLI students officially register at both DUT and UoL, and they can enjoy the excellent leaning resources and the student rights in both two leading universities.

During the past three years, both the management and academic teams of the Chinese and British side have been coordinating and innovating corporately to conglomerate the Chinese and British philosophy and resources for advantageous elite education. In the future, DLI will continue to develop towards the top-level international institute globally under the strong support of DUT and UoL for cultivating competitive talents with global vision.



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06July 2020

Dear Zlyu,

year expecting 70%, a first class per formance. This is something you should take considerable pride in. Of course this hasturned out to be a strange academic year and it's not yet dear how strange next academic year will be either! However, we will all get through this process and I can assure you that we will offer you an excellent level of teaching next academic year, come what may. You should be aware though that year 3 is a challenging year, as the complexity of the material continues to increase. However, your excellent performance in year 2 is a really good platform on which to build and if you work hard and stay or ganised you will continue to do well.

I hope you have a good summer break.

Yours sincerely

Drittena Piletaia, Head of Chemistry Year Two





# **DLI Students Achieve First Prize in the 2019 APMCM**

Source: Leicester International Institute, DUT



#### 2019 Asia and Pacific Mathematical Contest in Modeling

Awarded to

Certificate of Achievement

Dalian University of Technology

Yiyan Wang

xia mingxuan

Baochi Zhang

## First Prize

Undergraduate Group





Recently, the results of the 2019 Asia and Pacific Mathematical Contest in Modeling (APMCM) was announced. As an influential competition in the Asia-Pacific region, nearly 20,000 students from more than 500 universities attended this contest. 92 students from Leicester International Institute, Dalian University of Technology won different categories of prizes. Xia Mingxuan and Wang Yiyan were awarded the First Prize, which was the best result on DUT, Panjin campus and another top prize in the international mathematical

modeling competition for students besides the American Mathematical Modeling Competition.

The 2019 APMCM, organized by Beijing Society of Image and Graphics and undertaken by Mathematician (formerly Schoolyard Mathematical Modeling), aims to popularize mathematical modeling knowledge and exercise students' logical thinking skills in problem identification, problem analysis and problem solving in the information society. The questions and materials of the competition are in English. Students are required to solve

practical problems using numerical modelling methods and submit an English paper within 4 days. In the 2019 competition, the first prize accounts for 5%, the second prize accounts for 15% and the third prize accounts for 25%. At Dalian Leicester Institute, 2 students won the first prize, 5 students won the second prize, 28 students won the third prize and 57 students were awarded the honour of successful participants.

Xia Mingxuan and WangYiyan's team carried out a research on the topic "how to improve the regional economic vitality" from several aspects such as population, area, city, using MATLAB for data analysis. It analysed the influential factors for economic vitality in the method of linear fitting on the basis of least square, and got the ranking of urban economic vitality by gray correlation,

thus to solve the problem. Dalian Leicester Institute has been attaching great importance to students' scientific innovation ability and making great efforts to create strong scientific innovation atmosphere. It holds academic seminars and scientific sessions regularly to stimulate students' aspiration and interest on research. Meanwhile, the bilingual integration enables students to develop advantages and improve their competitiveness in international contests. Dalian Leicester Institute will keep encouraging students to participate in international scientific and innovative contests and providing platforms for students to expand their professional skills, cultivate their consciousness of innovation and cooperation and promote their all-round development.

