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Researcher of the Year 2019

Professor Enge Wang – A Legendary Researcher of Atomistic World

Dear Readers,

International Association of Advanced Materials (IAAM) proudly announces ‘Researcher of the year’ award every year to recognize the contribution of scientists towards the advancement of materials for global excellence. This year, the award is presented to eminent physicist Prof. Enge Wang, Vice President of Chinese Academy of Sciences (CAS) and President Emeritus of Peking University, China, for his contribution towards the nanotechnology research and innovations. He is one of the leading contributors in the field of surface physics; the approach is a combination of atomistic simulation of nonequilibrium growth and chemical vapor deposition of light-element nanomaterials.

Education and academic career

Prof. Enge Wang was born in Shenyang city of Liaoning province, China, in 1957 [1]. He majored in Physics in his graduation and postgraduation both from Liaoning University, China. He obtained his PhD in condensed matter physics from the Physics Department at Peking University, China. Wang went to the Physics institute of Chinese Academy of Sciences (CAS) and then moved to France and America for his post-doctorate research. In August 1995, he went back to China and was invited to be a CAS researcher. Meanwhile, he was the first young physicist who returned to China in the “100-Talent Program” of the CAS. He went on to serve as the Director of the Institute of Physics (CAS - Chinese Academy of Science) (1999-2007), Vice-President of Beijing University (2009-2013), the Provost and later as the President of Peking University (2011-2015), President of Beijing University (2013-15), the Vice President of CAS (2015-2017) and the Honorary Director of Kavli Institute for Theoretical Sciences at the University of CAS (2018) [2]. He has also served as the Vice President of the International Union of Pure and Applied Physics (IUPAP) and the International Council of American Physical Society (APS). He is a member of the World Academy of Sciences for the Advancement of Science in Developing Countries since 2008 and a fellow of the American Physical Society since 2006.

He joined as the 26th President of Peking University to succeed the former president Zhou Qifeng, who had become the president in November 2008 (Fig. 1). In his inauguration speech, Wang said that the university should have a dream - in the same way an individual or a country does [3].

“To build Beida into a world-class university is the dream of all people at the university,” he said. “But a school can prosper only through hard work, while empty talk will hinder our development.”



Fig. 1. Prof. Wang appointed as the 26th President of Peking University [3].

Awards and recognitions

Prof. Wang has been recognized with a number of international and national academic honors and awards for his excellent academic and research contributions: Outstanding Research Student Award (1988), Young Research Award (1996), Young Scientist Award (1997), Achievement in Asia Award (2003), IBM faculty Award (2003), National Science and Technology Awards (2004), The Third World Academy of Sciences Prize (2005), The Humboldt Research Award (2005), Outstanding Science and Technology Achievement Prize (2005), TWAS Award in Physics (2005), Best Invited Speaker (2007), Distinguished Lecturer (2007), The Stanford GCEP Scholar (2009), Distinguished Science and Technology Awards (2010), IMNI Distinguished Lectureship in Nanoscience (2012), Tan Kah Kee Science Award in Mathematics and Physics (2014) [4], and Advanced Materials Laureate (2018) being few of the most esteemed [5].

He has been elected to the Chinese Academy of Sciences and the World Academy of Sciences (TWAS). The CAS membership is the highest academic title and an honor of life tenure conferred by the state in science and technology circles in China. He has also been a part of various international physics committees, professional advisory committees, and editorial boards.

He has served as an Executive Editor of the international journal, AIP Advances.

Advanced Materials Laureate

International Association of Advanced Materials (IAAM) had the privilege to honor Prof. Enge Wang with the title of Advanced Materials Laureate 2018 during its 20th award assembly in Stockholm. It is considered as one of the highest honors for a researcher working in a diverse background (Fig. 2). During this assembly, Prof. Wang delivered Advanced Materials Laureate Lecture 2018 entitled, “*Water: Soft in Nature, Hard in Science*”.



Fig. 2. Professor Enge Wang was honoured with the prestigious Advanced Materials Laureate 2018 in the 20th assembly of IAAM Award Ceremony, Stockholm, Sweden [6].

In his Laureate talk, Prof. Wang summarized that “Despite water being a ubiquitous substance, it is surprising that some basic questions are still debated. Here, using a combination of experimental (cryogenic STM) and theoretical (first-principle electronic structures and molecular dynamics) methods, we systematically studied the unusual structure and dynamics of ice surface at atomic scale, and the sub-molecular imagining, clustering and proton transfer mechanisms of water on salt. First, an order parameter, which defines the ice surface energy, is identified. We predict that the proton order-disorder transition, which occurs in the bulk at ~ 72 K, will not occur at the surface at any temperature below surface melting. In addition, we find that the surface of crystalline ice exhibits a higher than expected concentration of vacancies at the external layer that may contribute to the phenomenon of pre-melting and quasi-liquid layer formation. Second, a STM molecular imaging mechanism based on a subtle control over the tip-molecule coupling is proposed, which allows a sub-molecular level resolution for water. A concerted proton tunneling mechanism is studied within the water tetramer, which is the basic unit to form an extended 2D ice layer by bridging water molecules on NaCl (001). These results shed light on our understanding of water at atomic scale” (Fig. 3).



Fig. 3. Watch [Advanced Materials Laureate Lecture 2018](#) (Video recorded by IAAM media), delivered by Prof. Wang on 21 August 2018 at Stockholm, Sweden.

Chinese Academy of Science (CAS) & Prof. Wang’s contribution in its development

CAS is a national scientific and academic body of China, headquartered in Beijing, and established in 1949, for natural sciences. It has about 104 research institutes, 12 branch academies, five universities, and 11 supporting organizations throughout the country [6]. It has also created hundreds of commercial enterprises with Lenovo being one of them. CAS has been associated with the development of science & technology throughout the nation and it also work as a think-tank giving advice and promoting research and also focuses on training young minds.

CAS is the world’s largest research organization and ranks among the top in the quality of research. Getting a CAS membership is the highest level of national honor for a Chinese scientist and the highest academic title in China. CAS members are obliged to advance science and technology and to promote international exchanges and cooperation. CAS scientists conduct research in both basic and advanced science & technologies and areas associated with public welfare and development of industries. CAS’s most recent achievements include breakthroughs in quantum computing, progress in superconductivity studies, stem cell research, and development in brain intelligence research.

Prof. Wang has been an academican of CAS since 1995. He started working as a Professor at the Institute of Physics, Chinese Academy of Sciences (CAS) and became the Vice President of CAS (2015-2017). He also chairs the Advisory Board of the Institute of Physics, CAS. In 2000, Prof. Enge Wang with Prof. Zhenyu Zhang and Prof. Earl Ward Plummer, founded the International Center of Quantum Structures (ICQS) at the Institute of Physics at Chinese Academy of Sciences. ICQS has produced many top Chinese physicists and fostered scientific collaborations, many of which have led to numerous influential research achievements.

In 2012, Prof. Wang edited a book series named “Peking University-World Scientific Advance Physics Series”, which covered many fields of modern Physics, such as condensed matter physics, optics, astrophysics, cosmology, particle physics, and mathematical physics.

The Series aimed to introduce significant achievements of Chinese physicists, both domestic and international, and to introduce the status of Chinese physics community to the international community.

Prof. Wang encouraged the CAS involvement through RADIS (The Institute of Remote Sensing and Digital Earth) and HIST (The International Center on Space Technology for Natural and Cultural Heritage) to provide support for the digital reconstruction and planning and monitoring of Preah Vihear Site, Cambodia, during his visit.

Contribution of Prof. Wang towards the advancement of materials to global excellence

Prof. Wang's research interest focuses on surface physics; kinetics of surface-based nanostructures, atomistic simulation, development of chemical vapor deposition of light element nanomaterials, and study of water on solid surface [7-20]. One of his main contributions is development of the Reaction-Limited-Aggregation (RLA) theory which is the opposite of the classic Diffusion-Limited-Aggregation (DLA) prediction model. It describes the morphological evolution of two-dimensional islands in the presence of a surfactant [21].

Prof. Wang and co-workers also predicted a three-dimensional Ehrlich-Schwoebel barrier; modelled atomic diffusion and produced novel nanostructure like tubular graphite cone and polymerized CN nanobells [22]. His work on the water-surface coupling and the strength of the hydrogen bonds at the interfaces provided a fundamental understanding of water on surface at molecular level. He also studied proton ordering and pre-melting of ice surface [23]. Recently, he examined water behaviours in confinement and proposed a two-dimensional tessellation ice [24]. His work on the water-surface coupling and the strength of the hydrogen bonds at the interfaces provided a fundamental understanding of water on surface at molecular level. He also studied proton ordering and pre-melting of ice surface [25].

Prof. Wang along with Dr. E.G. Wang, and Dr. Wengang Lu, utilized computational simulations methods; VASP, LMTO, KMC and *ab initio* Molecular Dynamics for studying theoretical aspects of their research. Mr. S. Liu and Dr. Xuedong Bai have been Prof. Wang's associates for experimental work utilising techniques for surface sensitive probes such as scanning tunnelling microscopy, high resolution electron energy spectroscopy, X-ray photoelectron spectroscopy, Auger electron spectroscopy, and low energy electron diffraction.

Prof. Wang has published over 300 high-quality publications including in top scientific journals *i.e.* in *Science*, *Nature*, *JACS*, *PRL*, *Co-editor of Books and MRS Proceedings*. Some of Prof. Wang's major research contributions are listed below:

In 2007, Prof. Wang and his team developed a method for the direct synthesis BCN (boron carbonitride)/C nanotube junctions [23]. The electrical

transport measurements of individual nanotube junctions were performed on a conductive atomic force microscopy and it was found that the BCN/C nanotube junction shows a typical rectifying diode behavior and this study got published in *JACS*.

In 2008, a new methodology for the controlled near-surface carbon doping of BNNTs was demonstrated by his team. Novel B-C-N/BN coaxial nanotubes were fabricated, and their *p*-type semiconducting behaviors were elucidated through gate-dependent transport measurements [10]. In addition, in the same year (2008), they published their research in *PRL*, explaining the surface of ice being significantly more proton ordered than the bulk [24]. They predicted that the proton order-disorder transition doesn't occur at the surface at any temperature below surface melting. They also identified a parameter defining the surface energy of ice.

Their team also explored theoretical research by undertaking *ab initio* simulation and density function theory calculations to study surface charge properties for fabricating nanomaterials [25-27] and another studied published in *PRL* showing the molecular dynamics and nuclear quantum studies to identify proton transfer and reorientation mechanism in BaZrO_3 [28].

Prof. Wang's team developed elastic graphene ribbons by continuous ripple creation of graphene on the surface of elastic substrate like polydimethylsiloxane (PDMS) films and published this data into *ACS Nano* [29]. These graphene ribbons are strain resistant and ideal for electronic applications.

A novel substitution reaction was developed for the synthesis of boron- and nitrogen-codoped single-walled carbon nanotubes (B(x)C(y)N(z)-SWNTs) in bulk quantities [30]. The as-synthesized ternary system B(x)C(y)N(z)-SWNTs are of high purity and quality and have homogeneous B and N-dopant concentrations. The B(x)C(y)N(z)-SWNTs were composed primarily of the semiconducting nanotubes (*JACS*).

In one of their study published in *Nature Communication* examined the They also discovered defects in the ferroelectric switching; the intrinsic electric fields formed at ferroelectric/electrode interfaces determine the nucleation sites and growth rates of ferroelectric domains and the orientation and mobility of domain walls, whereas dislocations exert a weak pinning force on domain wall motion by studying a tetragonal $\text{PbZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$ thin film under an applied electric field using *in situ* transmission electron microscopy [31]. They also identified a low temperature liquid state hydrogen using computer *ab initio* path-integral molecular dynamics (PIMD) methods, which are based on electronic structures computed as the dynamics of the system evolves and can account for bond formation and breaking in a seamless manner. They found a low-temperature metallic atomic liquid phase at pressures of 900 GPa and above, down to the lowest temperature. The identified atomic liquid is strongly quantum in nature, and the study provides a finite temperature phase diagram of hydrogen under ultra-high pressures and

gives direct numerical support for Ashcroft's low-temperature metallic liquid [15]. They further studied the finite temperature phase diagram of hydrogen in the region of phase IV and its neighborhood using the ab initio molecular dynamics (MD) and the ab initio path-integral molecular dynamics (PIMD) [18]. The electronic structures were analyzed using the density-functional theory (DFT), the random-phase approximation, and the diffusion Monte Carlo (DMC) methods. Comparing the energy differences from MD and PIMD simulation generated structures, it was revealed that standard functionals in DFT tend to underestimate the dissociation barrier of the weak molecular layers in the mixed phase. Because of this electronic structure generated leads to artificially dissociate hydrogen layers in phase IV. This analysis partly rationalizes why earlier ab initio MD simulations complemented the experimental observations so well. The temperature and pressure dependencies for the stability of phase IV were also studied in the end and compared with earlier results.

In 2015, his team reported the real time imaging of proton tunneling in a cyclic water tetramer using a cryogenic scanning tunneling microscope leading to a possibility of controlling the protons' movements at quantum level and published their research in Nature Physics [32]. They monitored the reversible interconversion of the hydrogen-bonding chirality of the water tetramer with a chlorine-terminated scanning tunneling microscope tip (Fig. 4). The presence of the Cl anion at the tip apex may either enhance or suppress the concerted tunneling process, depending on the details of the coupling symmetry between the Cl ion and the protons. Further, DFT calculations confirm the quantum nature of the proton transfer between the water molecules. The results show a visualization process of four protons tunneling in a concerted motion. The results formed a foundation for further work on water dynamics at quantum level leading to its unique properties.

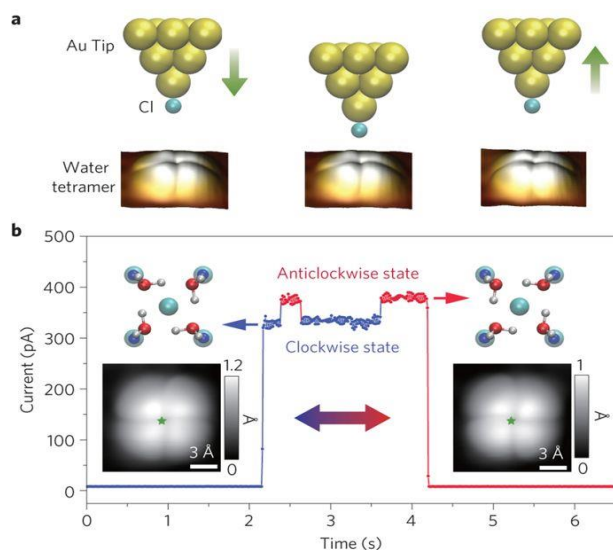


Fig. 4. Chirality switching of a H₂O tetramer (Reproduced with permission from [32]).

They developed a method for optical imaging and broadband in situ spectroscopy of individual carbon nanotubes on various substrates and in field-effect transistor devices using polarization-based microscopy combined with supercontinuum laser illumination [16]. The technique allows the complete chirality profiling of hundreds of individual carbon nanotubes, both semiconducting and metallic, on a growth substrate.

Another interesting development by Prof. Wang and team is the generation of large single crystal graphene sheet grown on copper foils with a growth rate of 60 $\mu\text{m s}^{-1}$ and size of 0.3 mm in just 5 s [19]. The high growth rate was achieved by placing the copper foil above an oxide substrate that provided a continuous supply of oxygen to the surface of the copper catalyst during the CVD growth, which significantly lowered the energy barrier to the decomposition of the carbon feedstock and increased the growth rate.

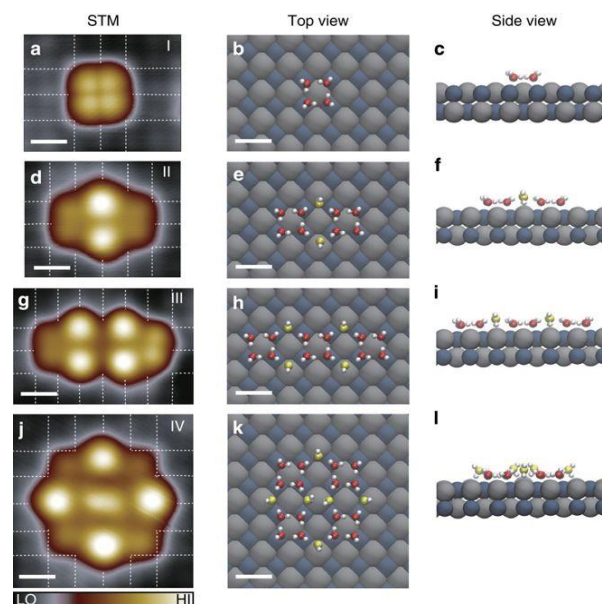


Fig. 5. Imaging and models of four types of water clusters (Reproduced with permission from [33]).

Prof. Wang has done some milestone work on water- solid interactions. His team gave a new model for water structure on an interface contradicting the widely accepted hexagonal bilayer model based on the Bernal-Fowler-Pauling ice rules [33]. This study was published in the journal, Nature Communications. They reported a two-dimensional ice like bilayer structure of cyclic water tetramers on a NaCl film, different from conventional bilayer (Fig. 5). This was achieved by using a cryogenic scanning tunneling microscope, to visualize individual water molecules adsorbed on an Au-supported NaCl (001) film. The bridging mechanism allowing water tetramers to form a 2D ice bilayer containing a regular array of Bjerrum D-type defect was revealed using ab initio DFT calculations. This structure with defect arrays must be responsible for catalyzing reactions on water-salt surface and influence phenomena like ice

nucleation, salt dissolution and caking. This strategy will help determining the detailed topology of H-bonded networks at water/solid interfaces with atomic precision.

Prof. Wang has contributed enormously as a scientist, educationist, academician, and researcher to the nanotechnology community by developing various novel nanomaterials. Prof. Wang had a habit of arriving at his office at 7:00 AM and leaving at 11:00 PM every day and this habit brought him a special nickname “711”, which was also the room number he had chosen for his office [34]. In his inaugural speech as the President of the Peking University, Prof. Wang said, “As a man, he must have a dream; as a country, it must have a dream; so, it is the same with a university. It is the very dream of the whole Peking University to build a world class university. Empty talks would lead the course astray, and hard work can rejuvenate the university. I will try my best to be a dedicated president and do what I am supposed to do with most passions and responsible spirit” [34]. Advanced Materials Letters feels very honored and privileged to confer upon him the ‘Researcher of the Year’ award for his several years of diligence and uncountable achievements in the field of nanomaterials.

We heartily congratulate Prof. Enge Wang for being recognized as the ‘Researcher of the year 2019’.

With kindest regards

Dr. Ashutosh Tiwari

Editor-In-Chief

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