Postprint Analysis of Nanotechnology Research Based on ESI Research Fronts

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Date: 2017-10-21T00:00:00+00:00

Abstract

The ESI database clusters to form research fronts based on co-citation relationships among highly cited papers (Top 1%). This study, based on 11,814 research fronts from the ESI database, identifies 1,391 research fronts in the nanotechnology domain through literature retrieval, expert selection, and other methods, and subsequently forms several research directions and research areas via manual clustering. Furthermore, it selects four research areas—solar cells, nano-bionic pores, nano-catalysis, and measurement and characterization—for in-depth analysis and interpretation, compares the number of highly cited papers across countries, and elucidates the research directions and teams where China possesses competitive advantages.

Full Text

Analysis of Nanoscience and Technology Development Based on ESI Research Fronts

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Abstract

The ESI database identifies research fronts in science through co-citation clustering, where each front consists of a group of highly cited papers (Top 1%) that have been co-cited above a set threshold of similarity strength, along with their associated citing papers. This paper identified 1,391 research fronts related to nanoscience and technology from the complete set of 11,814 research fronts in the ESI database through literature search and expert selection. These research fronts were further categorized into several research themes through expert identification. The analysis focused on four key research themes—solar cells, biomimetic nanopores, nanocatalysis, and measurement and characterization—comparing the performance of countries in producing highly cited papers and highlighting China' s advantageous research directions and leading research teams.

Keywords: research fronts, nanoscience and technology, solar cells, nanocatalysis, biomimetic nanopores

Since 2014, the strategic intelligence research team of the Chinese Academy of Sciences has collaborated with Clarivate Analytics (formerly the Intellectual Property and Science division of Thomson Reuters) to identify annual hot and emerging research fronts across ten major disciplinary fields from the ESI (Essential Science Indicators) database through bibliometric analysis and expert judgment. For three consecutive years, the team has published the *Research Fronts* annual report, which has generated positive responses from the scientific community and society [1]. The authors have led and participated in the development of these reports. While pleased with the achievements, we are also aware of two main limitations: (1) due to manpower constraints, the report can only analyze and interpret the most popular dozen or so research fronts in each disciplinary field, failing to provide a comprehensive analysis of the entire field; and (2) research fronts formed through bibliometric co-citation clustering are typically quite specific, focusing on research points (e.g., "polymer solar cells based on non-fullerene acceptors"), while revealing more macroscopic research directions (e.g., "polymer solar cells") remains to be improved.

Therefore, this paper selects nanoscience as a breakthrough case. Through literature search and expert selection, we identified all 1,391 research fronts belonging to the nanoscience research domain from the ESI database. First, through statistical analysis of highly cited papers published in these nanoscience fronts, we provide a macroscopic overview of the competitive landscape among countries. Then, based on the similarity of research topics, these research fronts were manually clustered into several research directions, which were further clustered into research domains, forming a three-level analysis structure of domain-direction-front (some domains have a four-level structure of domain-subdomain-direction-front). This analytical structure captures all research fronts involved in a research domain, enabling comprehensive, detailed, and in-depth analysis. Due to space limitations, this paper selected four domains for analysis and interpretation.

Selection of Nanoscience Research Fronts

The ESI database clusters highly cited papers (Top 1%) based on co-citation relationships to form clusters of highly cited papers. Each cluster includes several highly cited papers with the same or similar research topics, forming a "research front" [2]. The *Research Fronts* report is based on these research fronts from the ESI database. This paper started with the 11,814 research fronts in the ESI database and used the nanoscience search strategy constructed by Arora et al. [3] to first screen out 1,512 research fronts that might belong to the nanoscience domain. After expert selection and verification, 1,391 nanoscience research fronts were finally identified, involving 6,639 highly cited papers [4]. The ESI data were retrieved in January 2016, and the highly cited papers were published between 2008 and 2015.

Statistical analysis of the corresponding authors' countries for the 6,639 highly cited papers in nanoscience research shows that the United States and China rank first and second, respectively, far ahead of other countries, reflecting their overall strength in nanoscience research .

Solar Cells

The solar cell domain mainly includes perovskite solar cells, polymer solar cells, and quantum dot-sensitized solar cells, among other research directions, involving 102 research fronts and 516 highly cited papers. As shown in , the United States has the largest number of highly cited papers in this field, with China ranking second and showing a small gap with the United States. Other countries lag far behind in terms of highly cited paper numbers.

Perovskite Solar Cells Perovskite solar cells are the hottest research direction among third-generation solar cells. In just a few years, they have surpassed the achievements of new-generation thin-film batteries such as amorphous silicon, dye-sensitized, and organic solar cells that took more than a decade to develop. They were named one of the top ten scientific breakthroughs of 2013 by *Science* magazine. The core of perovskite solar cells is the organic-metal halide light-absorbing material with perovskite ABX3 crystal structure, with methylammonium lead iodide (CH3NH3PbI3) being the most common. In 2009, Miyasaka' s group at Yokohama University in Japan first used perovskite materials as the light-absorbing layer to create perovskite solar cells based on dye-sensitized solar cells, but the photoelectric conversion efficiency was only 3.8% [5]. In 2011, Nam-Gyu' s group at Sungkyunkwan University in South Korea increased the efficiency to 6.5% [6]. In 2012, Snaith' s group at Oxford University proposed the concept of "meso-superstructured solar cells," achieving a photoelectric conversion efficiency exceeding 10% for the first time [7]. In 2013, Grätzel' s group at EPFL in Switzerland increased the efficiency to 15% [8]. By the end of 2014, Seok' s group at the Korea Research Institute of Chemical Technology increased the conversion efficiency to 20.1% [9]. In 2015, a China-Japan-Switzerland collaboration produced large-area (working area exceeding 1 cm^2) perovskite solar cells, enabling them to be compared with other types of solar cells under the same standards for the first time, with a certified energy conversion efficiency of 15% [10]. In 2016, Grätzel' s group further increased the certified efficiency to 19.6% [11]. Compared with the United Kingdom, Switzerland, and South Korea, China has relatively fewer highly cited papers in this research direction.

Polymer Solar Cells In bulk heterojunction polymer solar cell research, fullerene-based materials have been the mainstream acceptor materials, but they have some prominent problems. To address this, researchers have developed non-fullerene acceptor materials, mainly including two categories: organic small molecules and polymers. In terms of organic small molecule acceptor materials, Zhan Xiaowei' s team at Peking University first proposed the concept of fused-ring electron acceptors and designed and synthesized a series of high-performance organic fused-ring electron acceptor materials, achieving a battery efficiency of 9.6% in 2016 [12]. In the same year, Hou Jianhui's team at the Institute of Chemistry, Chinese Academy of Sciences, using organic small molecule acceptors, achieved a record-breaking energy conversion efficiency of 11.2% in small-area non-fullerene polymer solar cell devices, bringing the efficiency of non-fullerene polymer solar cells to the level of fullerene acceptors [13]. In terms of polymer acceptor materials, i.e., all-polymer solar cells, Li Yongfang' s team at the Institute of Chemistry, Chinese Academy of Sciences, has been active. In 2016, the team increased the energy conversion efficiency of all-polymer solar cells to 8.27% [14]. Additionally, in 2016, Chen Yongsheng's team at Nankai University used a complementary light absorption strategy with oligomer materials to construct a tandem organic solar cell device with broad-spectrum absorption characteristics, achieving a photoelectric conversion efficiency of 12.7%, which set the highest recorded efficiency for organic/polymer solar cells at that time [15].

Quantum Dot-Sensitized Solar Cells Quantum dot-sensitized solar cells have attracted widespread attention in recent years due to their low preparation cost, simple process, and the excellent properties of quantum dots themselves (such as size effects and multiple exciton generation). Sargent' s group at the University of Toronto in Canada [16], Nozik' s group at the National Renewable Energy Laboratory in the United States [17], and Zhong Xinhua' s team at East China University of Science and Technology [18] have been particularly prominent in this area. In 2016, Zhong Xinhua' s team increased the photoelectric conversion efficiency of quantum dot-sensitized solar cells to 11.61%, which was certified by the National Center for Photovoltaic Quality Supervision and Testing [19].

Biomimetic Nanopores

The biomimetic nanopore domain mainly includes biological nanopores and solid-state nanopores, involving 5 research fronts and 45 highly cited papers. As shown in , the United States has a very significant research advantage in this field, with 23 highly cited papers, more than half of the total. The United Kingdom and Germany rank second and third, respectively, while China has only one highly cited paper.

In the 1990s, scientists proposed the idea of pulling single-stranded DNA through protein pores to detect tiny changes in conductance as bases pass through, thereby achieving nanopore DNA sequencing. Entering the 21st century, more and more researchers have dedicated themselves to this field, making nanopore sequencing a reality, with research results gradually moving toward commercial practicality. Our analysis shows that the types of nanopores involved in highly cited papers mainly include biological nanopores and solid-state nanopores, with sequencing mainly including nucleic acid sequencing (primarily DNA sequencing) and protein analysis.

Biological nanopores refer to nanopores that utilize natural biological channels (such as -hemolysin structures, Mycobacterium smegmatis porin A (MspA), etc.). Oxford Nanopore Technologies' Hagan Bayley team developed a commercializable -hemolysin biological nanopore. In 2009, the company achieved continuous base determination with an average accuracy of 99.8% [20]. Subsequently, Oxford Nanopore Technologies launched commercial nanopore sequencers—MinION and GridION. The single-molecule DNA reading technology based on nanopores no longer requires optical detection and synchronized reagent elution processes and is also known as fourth-generation sequencing technology, which has faster data reading speeds and greater application potential than earlier sequencing technologies. In 2016, MinION successfully completed DNA sequencing under microgravity conditions on the International Space Station and was named one of the top ten scientific breakthroughs of the year by *Science*.

In 2010, Gundlach at the University of Washington first demonstrated that MspA could be used for DNA sequencing and collaborated with microbiologist Michael Niederweis at the University of Alabama to prove that MspA pores combined with a "ratchet system" could read short DNA sequences [21]. In 2012, the team used MspA and bacteriophage phi29 polymerase to achieve single-nucleotide resolution and DNA translocation control, addressing two major obstacles that biological nanopores had long encountered [22]. In the same year, Mark Akeson' s team at the University of California, Santa Cruz, also used MspA and phi29 polymerase to achieve real-time detection of single nucleotides with DNA forward and reverse ratcheting at speeds of 2.5–40 nucleotides per second [23].

Biological nanopores have limitations in stability and durability, making it difficult to meet the needs of continuous large-scale sequencing. With the continuous advancement of microfabrication technology, solid-state nanopores have emerged. Artificially prepared solid-state nanopores have the advantages of stable pore size, good physicochemical properties, low cost, high read length, and easy integration, and are considered the next generation of nanopore technology. The materials for solid-state nanopores mainly include graphene, silicon nitride, silicon, and metal oxides.

Graphene has excellent potential for DNA detection. In 2010, Golovchenko' s team at Harvard University and researchers at MIT published a paper in *Nature* demonstrating that graphene could be made into artificial membrane materials for DNA sequencing, pointing the way for graphene nanopore DNA detection [24]. Golovchenko' s team prepared graphene nanopores that closely match the diameter of DNA molecules and found that they have very good sensitivity and resolution for DNA [24]. At the same time, the detection range of nanopores has continuously expanded, from DNA to RNA, proteins, gold nanoparticles, and toxic molecules. For example, Hagan Bayley' s team at Oxford Nanopore Technologies, Mark Akeson' s team at the University of California, Santa Cruz, and Cees Dekker' s team at Delft University of Technology in the Netherlands have used biological nanopores for protein detection [25]; Marija Drndić and Meni Wanunu' s team at the University of Pennsylvania used thin nanopores to rapidly detect small RNA molecules [26]; researchers at the University of East Anglia in the UK used MinION sequencing to identify the position and structure of bacterial antibiotic resistance islands [27].

Nanocatalysis

The nanocatalysis domain mainly includes subdomains such as catalyst synthesis and preparation, traditional catalysis, electrocatalysis, and photocatalysis, involving 92 research fronts and 303 highly cited papers. Catalyst synthesis and preparation mainly includes research directions on active components and supports; traditional catalysis mainly includes C1 catalysis; electrocatalysis mainly includes fuel cells, water electrolysis, and CO2 conversion; photocatalysis mainly includes degradation of pollutants in water and air, CO2 conversion, and water splitting. As shown in , China ranks first in the number of highly cited papers in this field, with a share exceeding one-third, reflecting China' s strong research advantage in nanocatalysis in recent years. The United States ranks second, with a share close to one-quarter. Other countries have relatively few highly cited papers.

Nanocatalysts typically consist of two parts: active components and supports. Common active components include metals (and their compounds), semiconductors, and carbon-based materials (such as graphene, carbon nanotubes, and graphitic C3N4). Size, morphology, structure, and composition are important factors affecting the catalytic utility of active components. For cost considerations, the overall research trend for active components is to use abundant and inexpensive common metals or non-metal materials to replace precious metals while ensuring activity. Common supports include oxides (such as SiO2, TiO2, and Fe3O4), carbon-based materials (such as graphene, carbon nanotubes, and graphitic C3N4), and porous materials (such as zeolites, mesoporous materials, and metal-organic frameworks). Supports not only provide surfaces for the high dispersion of active components but can also participate in the catalysis process, such as promoting photogenerated charge separation. For porous supports, the confinement of pore channels can play a shape-selective catalytic role. Due to easy separation and recovery, magnetic recoverable supports have developed rapidly in recent years. Zhang Tao' s team at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, first discovered that single-atom catalysts have activity comparable to homogeneous catalysts, experimentally demonstrating that single atoms may become a bridge between homogeneous and heterogeneous catalysis [28].

Nanocatalysis reactions are roughly divided into three categories: traditional catalysis, electrocatalysis, and photocatalysis.

In traditional catalysis, C1 chemistry occupies an important position, including Fischer-Tropsch synthesis, methane conversion, CO oxidation, CO2 reduction, and methanol oxidation. In recent years, China has made a series of major breakthroughs in C1 chemistry. Bao Xinhe’ s team at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences, constructed a single-center iron catalyst confined in a silicide lattice, successfully achieving selective activation of methane under oxygen-free conditions to efficiently produce high-value chemicals such as ethylene, aromatics, and hydrogen in one step [29]. Bao Xinhe’ s team also used a self-developed new composite catalyst to creatively convert syngas from coal gasification directly into low-carbon olefins with high selectivity, with selectivity for ethylene, propylene, and butene exceeding 80%, breaking through the 58% limit of Fischer-Tropsch synthesis for low-carbon olefins and changing the history of more than 90 years of relying solely on the Fischer-Tropsch route [30]. A joint research team from the Shanghai Advanced Research Institute, Chinese Academy of Sciences, and ShanghaiTech University independently developed a Co2C nano-hexahedral structure catalyst with exposed {101} and {020} crystal facets, achieving high-selectivity direct preparation of olefins from syngas under mild conditions (250°C, 1-5 atm), with selectivity for low-carbon olefins reaching 60%, total olefin selectivity up to over 80%, and an olefin/alkane ratio as high as over 30 [31].

In electrocatalysis, the oxygen reduction reaction at the cathode of fuel cells and metal-air batteries is one of the research focuses. Platinum is an important electrocatalyst for the oxygen reduction reaction. Due to the high cost of platinum, catalyst development is moving in two directions: one is to reduce platinum usage by using binary or ternary alloys, such as Pt-Fe, Pt-Co, and Pt-Fe-Cu; the other is to develop non-platinum catalysts, such as palladium and its alloys, and nitrogen-doped carbon materials (such as graphene and carbon nanotubes). Water electrolysis is another important electrocatalytic reaction. New hydrogen evolution catalysts include molybdenum sulfide compounds (such as MoS2 and MoS3) and metal catalysts encapsulated in nitrogen-doped carbon nanotubes, while new oxygen evolution catalysts include nitrogen-doped graphene. Hongjie Dai’ s team at Stanford University prepared a Co3O4/nitrogen-doped graphene electrocatalyst with high activity for both oxygen reduction and oxygen evolution, attracting strong attention, with the paper being cited more than 2,000 times [32]. CO2 conversion catalysts are also a research hotspot. Yi Xie’ s team at the University of Science and Technology of China used a new cobalt-based electrocatalyst to efficiently and cleanly convert CO2 into liquid fuel, receiving high praise from international peers [33].

In photocatalysis, the degradation of pollutants in water and air is one of the research focuses. Common catalysts include semiconductors such as TiO2, BiOX (X = Cl, Br, I), Ag/AgX (X = Cl, Br, I), and graphitic C3N4. The reduction of CO2 to produce CH4, CH3OH, and other hydrocarbon fuels is a current research hotspot, which can provide alternative energy while reducing greenhouse gases. Common catalysts include semiconductors such as TiO2, Ag/AgX (X = Cl, Br, I), metal-organic frameworks, graphene, and graphitic C3N4. Photocatalytic water splitting has always been an important topic in photocatalysis. The graphene-loaded CdS photocatalyst for hydrogen production prepared by Jianru Gong at the National Center for Nanoscience and Technology and Jiaguo Yu at Wuhan University of Technology has attracted high attention, with the paper being cited more than 1,000 times [34].

Measurement and Characterization

The measurement and characterization domain mainly includes super-resolution optical microscopy, nanoscale magnetic resonance research, and electron microscopy measurement, involving 39 research fronts and 153 highly cited papers. As shown in , the United States has the largest number of highly cited papers in this field, with Germany and the United Kingdom ranking second and third, respectively. China ranks fourth, with a significant gap in paper numbers compared to the United States.

Super-Resolution Optical Microscopy With the rise of super-resolution fluorescence microscopy in recent years, researchers have developed various super-resolution optical microscopes that break the diffraction limit, achieving resolutions of about 20 nm, and in some cases even less than 2 nm. These super-resolution microscopes are mainly divided into two categories: one is represented by the stimulated emission depletion microscope (STED) invented by Stefan Hell, which achieves super-resolution by modulating the illumination method; the other is based on single-molecule localization, which achieves super-resolution by imaging and localizing fluorescent groups with photoswitching functions. Photoactivated localization microscopy (PALM), stochastic optical reconstruction microscopy (STORM), and fluorescence photoactivation localization microscopy (fPALM) are all research hotspots in this direction. The 2014 Nobel Prize in Chemistry was awarded to three scientists for developing super-resolution fluorescence microscopy: Eric Betzig from the Howard Hughes Medical Institute (PALM technology), Stefan W. Hell from the Max Planck Institute for Biophysical Chemistry (STED technology), and William E. Moerner from Stanford University.

Nanoscale Magnetic Resonance Current conventional magnetic resonance spectrometers are limited by detection methods to millimeter-level imaging resolution. Nanoscale weak magnetic detection technology has advanced magnetic resonance research objects to single molecules and improved imaging resolution to the nanoscale. In 2008, Wrachtrup' s team at the University of Stuttgart and

Lukin’ s team at Harvard University first reported the use of nitrogen-vacancy centers in diamond for nanoscale weak magnetic detection, pioneering the research direction of nanomagnetometry [35]. Additionally, Yacoby’ s team and Walsworth’ s team at Harvard University, as well as Jiangfeng Du’ s team at the University of Science and Technology of China, have been very active in this direction. Du’ s team has achieved major breakthroughs such as the vector reconstruction of microwave fields with hundred-nanometer resolution and the mapping of the world’ s first magnetic resonance spectrum of a single biological molecule [36].

In-Situ Electron Microscopy In-situ transmission electron microscopy (in-situ TEM) technology enables dynamic, real-time observation of the microstructural response behavior of materials under external stimuli. Jianyu Huang’ s team at Sandia National Laboratories (who has since joined Yanshan University full-time) used in-situ TEM technology to characterize the lithiation and delithiation processes of nano-electrode materials in real time, achieving for the first time the construction of a lithium-ion battery system under a transmission electron microscope to study the morphological changes of nanowires during lithiation and the lithiation mechanism as lithium-ion battery electrodes [37].

Conclusions

Through bibliometric analysis of the nanoscience domain combined with domain intelligence research, this paper draws the following conclusions:

1. Based on the 11,814 research fronts in the ESI database from Clarivate Analytics, 1,391 research fronts related to nanoscience research were identified through literature search and expert selection, involving 6,639 highly cited papers (2008-2015). In terms of highly cited paper numbers, the United States and China rank first and second, respectively, far ahead of other countries.
2. The 1,391 nanoscience research fronts were manually clustered into several research directions and domains. Four domains were selected for analysis and interpretation: solar cells, biomimetic nanopores, nanocatalysis, and measurement and characterization. In terms of highly cited paper numbers, the United States ranks first in solar cells, biomimetic nanopores, and measurement and characterization, and second in nanocatalysis. China ranks first in nanocatalysis, second in solar cells, fourth in measurement and characterization, and does not rank in the top tier for biomimetic nanopores.
3. China has formed a number of world-leading research directions and excellent teams in nanoscience and technology. For example, in solar cells: Li Yongfang’ s team at the Institute of Chemistry, Chinese Academy of Sciences; Hou Jianhui’s team at the Institute of Chemistry, Chinese Academy of Sciences; Zhan Xiaowei’ s team at Peking University; Chen Yongsheng’

s team at Nankai University; and Zhong Xinhua’ s team at East China University of Science and Technology. In C1 chemistry: Bao Xinhe’s team at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences; and the joint research team from the Shanghai Advanced Research Institute, Chinese Academy of Sciences, and ShanghaiTech University.

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