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Materials Science at Beihang: A Special Issue of *Materials Lab* Dedicated to the 70th Anniversary of Beihang University

Li-Dong Zhao*, Hongbo Guo* and Chengbao Jiang*

This special issue is a collection of perspectives by the faculty members from School of Materials Science and Engineering at Beihang University to celebrate the 70th Anniversary of Beihang University.

Founded on October 25, 1952, Beihang University, or Beijing University of Aeronautics and Astronautics (Chinese: 北京航空航天大学), is a merger of eight aeronautics departments of Tsinghua University, Peiyang University (now known as Tianjin University), Xiamen University, Sichuan University, Yunnan University, Northwestern Institute of Engineering (now known as Northwestern Polytechnical University), School of Engineering of North China University (now known as Beijing Institute of Technology), and Southwest Industrial College (now known as Chongqing University). Beihang is the first university in China focusing on aeronautical and astronautical education and research, also covering diverse fields in the natural sciences, high technology, economics, management, the liberal arts, law, philosophy, foreign languages and education.

School of Materials Science and Engineering at Beijing University was founded in 1954 as the Department of Aeronautical Metallurgy. In 2001, it was named School of Materials Science and Engineering, consisting of Department of Materials Science, Department of Materials Physics and Chemistry, Department of Materials Processing Engineering and Automation, and Department of Polymer and Composite Materials. The discipline of Materials Science and Engineering is ranked as the first national key discipline during the first batch of evaluation by China Discipline Ranking (CDR). The development goal of the discipline is "Keeping the characteristics of Aerospace and Aeronautics, Meeting the national strategic demands, Leading the frontier of discipline, and Building up a world first-class discipline".

This special issue covers a broad range of cutting-edge research in materials science, including energy materials, metal materials, magnetic materials, computational materials, and advanced functional materials. It represents the university's new emerging and developing directions in materials science.

The perovskite solar cells (PSCs) based on carbon electrode (C-PSCs) are expected to address the instability issues faced by conventional PSCs. Recently, inorganic perovskites have been widely used as the light absorber in C-PSCs, which tended to further enhance device stability. Among various inorganic perovskites, $CsPbI_3$ perovskite has been showing the greatest promise due to its suitable band gap (~1.7 eV) and high chemical stability. Benefiting from the progress in phase stability, crystal quality and surface defect passivation, $CsPbI_3$ C-PSCs have achieved efficiencies of over 15% and exhibited considerable enhancement in device stability. Herein, Prof. Haining Chen (陈海宁) highlighted the main advances on $CsPbI_3$ C-PSCs and the future research directions.[1]

Owing to the high theoretical specific capacity and low electrochemical potential, lithium (Li) metal is considered as the most promising anode material for next-generation batteries. However, the commercial application of lithium metal batteries (LMBs) is restricted by Li dendritic growth and infinite volume change. Generally, introducing lithiophilic sites and constructing artificial solid-electrolyte interphase (SEI) layer are regarded as effective ways to induce uniform deposition of Li and inhibit the growth of Li dendrites. Herein, Prof. Yongji Gong (宫勇吉) summarized the current progress of 2D materials for LMBs, focusing on constructing lithiophilic sites and artificial SEI layers. Perspectives on future directions for LMBs are discussed.[2]

Thermoelectric (TE) materials and their devices have practical and potential applications for both power generation and electronic cooling in the fields of aerospace, weaponry, industrial waste heat recovery, 5G chip refrigeration, civil facilities, etc. The further and large-scale application of TE technology is dramatically limited by its conversion efficiency, determined by the dimensionless figure of merit (*ZT*). Tuning carrier concentration is the most basic but essential step for achieving high *ZT* values. Generally, at low carrier concentrations (< 10^{19} cm^{-3}), poorer electrical transports would result in inferior thermoelectric properties. Herein, Prof. Li-Dong Zhao (赵立东) proposed that potential high *ZT* values might also be obtained at lower carrier concentrations of ~10^{18} cm^{-3} by boosting carrier mobility.[3]

Jet engines are vulnerable to contamination by environmental debris (volcanic ash, sand and dust, referred to as

School of Materials Science and Engineering, Beihang University, Beijing 100191, China

* Corresponding author, E-mail: zhaolidong@buaa.edu.cn; guo.hongbo@buaa.edu.cn; jiangcb@buaa.edu.cn

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CMAS). When CMAS ash is ingested into gas turbines, it melts and can adhere to hot components of the jet engines, which may clog engine parts and attack protective ceramic thermal barrier coatings (TBCs). In excess cases, this contamination may endanger engine performance, and can even cause catastrophic failure. Prof. Hongbo Guo (郭洪波) and Wenjia Song (宋文佳) presented the current understanding of these CMAS issues in nature and deposit-induced failure mechanisms of TBCs. Details of experimental and theoretical analysis of the melting and impacting processes of CMAS ash in jet engines, and the strategy mitigation of new functional thermal barrier coatings to prevent the wetting of CMAS are described.[4]

The concept of "metastability engineering" has been successfully used in metallic structural materials to enhance mechanical properties. Prof. Wenlong Xiao (肖文龙) proposed that metastability engineering strategy can be introduced to Titanium alloys by destabilizing the β phase and taking advantage of metastable phase mediated phase transformation and twinning. The utilization of metastability engineering strategy and associated structural and functional properties of Titanium alloys are outlined.[5]

High entropy alloys (HEAs) have emerged as a new class of materials that can exhibit superior mechanical properties to the conventional alloy systems. Therefore, they are promising candidates as the next-generation structural materials. As the studies into the HEAs deepen, the original proposal of equal concentration of each element while remaining a single phased structure has been expanded and new opportunities start to emerge. Prof. Shiteng Zhao (赵士腾) and Prof. Zezhou Li (李泽洲) briefly discuss several future directions for HEAs which include fundamental questions such as chemical short-range order and synergistic strengthening mechanisms, as well as HEA's potential applications under extreme conditions such as high-temperature load-bearing, impact protection and kinetic penetrator.[6]

With the development of aerospace technology, the performance of equipment has been faced with new requirements and challenges. To ensure the safety service of aerospace equipment, it is urgent to find out the failure mechanisms and improve the service performance and life of key structural materials. Aluminum alloys are widely used as structural materials in aerospace field. Corrosion-induced failure is one of the most important failure modes. Studying corrosion mechanisms and developing new protective materials and methods are essential for the safety and long service life of aerospace aluminum alloys. Prof. Mei Yu (于美) discussed the corrosion resistance improvement by modifying the substrate matrix, the coatings, and the bonding force between the substrate and the coatings, providing an in-depth perspective on the specific corrosion status and potential corrosion problems of aluminum alloys.[7]

Antiferromagnetic spintronics is one of the leading candidates for next-generation electronics. Among abundant antiferromagnets, noncollinear antiferromagnets are promising for achieving practical applications due to coexisting ferromagnetic and antiferromagnetic merits. Prof. Zhiqi Liu (刘知琪) briefly reviewed the recent progress in the emerging noncollinear antiferromagnetic spintronics from fundamental physics to device applications. Current challenges and future research directions for this field are also discussed.[8]

The launching integrated computational materials engineering and materials genome engineering has led the transformation of empirical and theoretical design paradigms into the rational computational one that further provides the basis for the data-driven design paradigm, and ultimately enabling the possibility of materials intelligence design (MID) via artificial intelligence. Prof. Ruifeng Zhang (张瑞丰) highlighted the intelligent solution to acquire the property-structure-process-performance relationship of multilevel-structured materials by emphasizing modularization, automation, standardization, integration and intelligence, following the hierarchical relationship of data, information, knowledge and wisdom. The new era of MID is expected to fundamentally reform the material innovation mode through an integrated infrastructure guided by novel concepts that is radically distinguished from the way of thinking and doing in the past.[9]

Featuring high specific capacity, low cost, and environmental benignity of sulfur, lithium-sulfur batteries (LSBs) have been regarded as a promising candidate for the next generation of high-performance energy storage conversion and storage techniques with carbon-neutral capability. Nevertheless, technological challenges arising from both sulfur (S) cathode and lithium (Li) anode prevented the practical application of LSBs. Nowadays, theoretical models play an increasingly important role in Li-S systems in probing highly catalytic cathodes and dendrite-free anodes as well as exploring the conversion reaction mechanism. Prof. Qianfan Zhang (张千帆) reviewed the LSBs theoretical research projects, highlighting the interpretation and guidance of ab-initio simulations on experiments. They also presented the prospect of combining automatic workflow managers with ab-initio simulations in the development of LSBs.[10]

Semiconducting quantum dots (QDs) received considerable attention for application in optoelectronic devices, such as solar cells, photodetectors and light-emitting diodes, due to their unique fundamental properties, including solution processability, size-dependent bandgap energies, high stability and low cost. Specifically, the suitable bandgap energy of QDs with strong light absorption in the visible and near-infrared regions makes them a kind of competitive photovoltaic material toward next-generation photovoltaics. Herein, Prof. Xiaoliang Zhang (张晓亮) highlighted the advantages of emerging QDs, including infrared lead sulfide QDs and perovskite QDs for new generation photovoltaics, and the possible challenges and opportunities approaching high-performance solar cells are also proposed.[11]

Liquid crystal elastomers (LCEs) are a type of responsive materials combining liquid crystal mesogens with polymer networks. The LCEs exhibit outstanding actuation performance responsive to multiple external stimuli and show great potential as soft actuators. However, compared with conventional soft actuators, the LCEs need to be carefully synthesized and a few fabrication methods have been developed. Herein, Prof. Zhijian Wang (王志坚) and Prof. Jiping Yang (杨继萍) highlighted the strategies for the material design and manufacturing techniques. Several recent studies on the mechanical design for soft LCE actuators are overviewed. They further discussed the challenges and future perspectives of the LCE based actuators for soft robots.[12]

Creating brain-like devices that emulate how the brain

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works and can communicate with the brain is crucial for fabricating highly efficient computing circuits, monitoring the onset of diseases at early stages, and transferring information across brain-machine interfaces. Simultaneous transduction of ionic-electronic signals would be of particular interest in this context since ionic transmitters are the means of information transfer in human brain while traditional electronics utilize electrons or holes. Prof. Haitian Zhang (张海天) proposed strongly correlated oxides as potential candidates for this purpose. They discussed the mechanism behind the interplay between ionic doping and the resistivity modulation in perovskite nickelates and presented case studies of using the perovskite nickelates in neuromorphic computing and brain-machine interface applications, providing exciting new opportunities for future computation devices and brain-machine interfaces.[13]

Fe–N–C catalysts have the potential to replace the costly platinum catalysts in fuel cells but face the challenge of instability. It is of vital importance to identify the chemical nature of durable active sites in Fe–N–C. Prof. Jianglan Shui (水江澜) analyzed the geometric and electronic factors that affect the intrinsic durability of the FeN_xC_y moieties and proposed that iron–oxygen binding energy is most relevant. They then propose the iron oxidation (valence) state as an apparent descriptor of the Fe–O binding strength. Their proposal will deepen the understanding of the activity–stability trade-off for Fe–N–C catalysts and guide future active site optimization.[14]

Low-symmetry 2D materials, such as black phosphorus (BP), ReS_2, etc., usually exhibit unique characteristics of its in-plane anisotropy. Inspired by this, the searching for novel low-symmetry 2D materials beyond BP and ReS_2 is essential for creating polarization dependent devices and will benefit the future explorations of heterojunction on low-symmetry 2D materials. Prof. Shengxue Yang (杨圣雪) reviewed the research on structure, characterization and applications of low-symmetry 2D materials his group participated in.[15]

Two-dimensional (2D) charge density wave (CDW) materials have attracted widespread attention due to their exotic physical properties. Compared to their bulk forms, 2D CDW materials exhibit many excellent features, offering new possibilities for electronic device applications. Prof. Chen Si (司晨) highlighted the unique advantages of 2D CDW materials and identify some key challenges which remain to be addressed.[16]

We deeply appreciate *Materials Lab* provides a good opportunity to organize this special issue. We also want to show our deep appreciation to our colleagues from school of materials science and engineering for their contributions to this special issue. We sincerely hope that this special issue could present to readers Beihang's recent research advances in materials science.

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Biographies

Li-Dong Zhao is a full professor of the School of Materials Science and Engineering at Beihang University, China. He received his Ph.D. degree from the University of Science and Technology Beijing, China in 2009. He was a postdoctoral research associate at the Université Paris-Sud and Northwestern University from 2009 to 2014. His research interests include electrical and thermal transport behaviors in the compounds with layered structures. He has authored over 250 peer-reviewed publications in international journals with an h-index of 75. Professor Zhao has been identified as Highly Cited Researchers by Clarivate (2019-2021).

Hongbo Guo is a Professor at School of Materials Science and Engineering, Beihang University, and Director of Key Laboratory of High-Temperature Structure Materials and Protective Coatings (Ministry of Industry and Information Technology). Professor Guo had earned his Ph.D. degree in Beihang University. He has worked on high-temperature protective coatings for superalloys and ceramic matrix composites (CMC). He has published more than 200 research papers in International Journals and owned more than 60 granted patents. He had co-chaired ECI International Thermal Barrier Coatings Conferences which were held in Germany. Also, He had chaired the symposiums of Surface Coatings & Technology in 2010, 2013 and 2015 International Conference of Advanced Materials organized by International Union Materials Research Society (IUMRS-ICAM).

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Chengbao Jiang is a full professor of the School of Materials Science and Engineering at Beihang University, China. He received his bachelor's degree from Hefei University of Technology, China in 1990, and his Ph.D. degree in University of Science and Technology Beijing, China in 1996. Subsequently, he entered Beihang University and work until now. He has served as the Dean of School of Materials Science and Engineering at Beihang University, China since 2014. His research interests include magnetic functional materials and devices, advanced solidification theory, crystal growth, etc. He was honored with the first prize of National Technical invention (rank 2, 2008), the second prize of National Natural Science (rank 1, 2017), etc.